3.1 INTRODUCTION

D. J. Klein and M. Randic [1] invoked the theory of resistive electrical networks to develop a novel concept; if the fixed resistance is assigned to each edge of a connected graph, then the effective resistance between pairs of vertices is a graphical distance. Buckley and Harary [2] in their book distances in graphs define the graphical distance as minimal sum of positive edge weights along a path between the two sites (vertices). However the authors [1] developed the field of graph theory through the application of resistive electrical networks and mathematical chemistry. For example in chemistry different multiplicity bonds are distinct so that the associated edge weights are ordered inversely to the bond multiplicities. If the multiple bonds indicate shorter distance then multiple shortest paths between two well separated vertices (nodes or atoms) might indicate shorter chemical distance. According to new concept of resistance distance we imagine fixed unit resistor on each edge of a connected graph. Then the resistance distance between two vertices is defined as the effective resistance between two vertices when a battery is connected across them. Hence this new distance function has the characteristic of multiple route distance diminishment.

The RD (resistance distance) between any pair of vertices i
and \( j \) of a graph (or its equivalent network) when unit resistors are placed on each edge, will be denoted by \( r(i, j) \). The resistance of the graph \([3]\) \( R(G) \) is defined as the sum of RD's between all pairs of vertices.

\[
i.e., \quad R(G) = \sum_{i<j} r(i, j) \tag{3.1}
\]

The value \( R(G) \) is a graph invariant. The possibility of chemical utility of \( R(G) \) of a molecular structure is expected, since the conventional distance between nodes (atoms) has found several uses in chemistry. It is important to note that \( R(G) \) akin to well known Wiener number \( W(G) \). In case of acyclic molecular structure \( R(G) \) is identical with \( W(G) \), while in molecular structures containing cycles \( R(G) \) and \( W(G) \) are different. In this present chapter we have developed some results with acyclic molecular structures and their resistances.

### 3.2 MOLECULAR GRAPHS AND RESISTANCE DISTANCE

The concept of molecular graph was first introduced by Sir Arthur Cayley [5,6,7] in 1847. He considered two types of molecular graphs. In the first type all atoms (i.e., both carbon and Hydrogen) are represented by vertices and are called plerograms. In the second type hydrogen atoms are suppressed and only carbon atoms were considered to draw the graphs and these graphs called kenograms. Vast majority of Books and research papers use the term molecular graph mean to kenograms as they have smaller number of vertices and significantly simpler structure compared to plerograms. In most of the applications
kenogram structure representation is mathematically equivalent to plerogram structure representation and therefore kenogram is more convenient from practical point of view.

For example consider the following molecular graphs.

![Plerogram and Kenogram](image)

Fig. 3.1

Figure 3.1 Two graph representation of the same organic molecule viz., 2-2-3-5 tetramethylhexane

In Plerogram both carbon and hydrogen atoms are shown with total number of vertices is 32 (=3n+2), where n is the number of carbon atoms.

In kenogram hydrogen atoms are suppressed and only carbon atoms are considered. Note that the number of vertices of molecular graph is equal to the number of carbon atoms. In the above example n = 10.

Analogous to the above example, one can draw the acyclic graph for carbon atom skeleton of molecular structures, in the form of kenogram. Thus Figure 3.2 represents the molecular graph (carbon atom skeleton) of 2-4-4 trimethylheptane.
Fig. 3.2 Graph G

Molecular graph (G) of 2-4-4 trimethylheptane.

Let G be a graph and let its vertices be labeled by 1, 2, 3, \ldots n. These vertices form a path in the graph. The length of the shortest path that connects the vertices u and v is called the distance between the vertices and is denoted by d(u, v). Similarly, the resistance distance r(u, v) between vertices u and v is the effective resistance between u and v when unit resistors are assigned on each edge of the graph.

Consider the molecular graph of the Figure 3.2. The resistance distances between all pairs of vertices are listed below.

\begin{align*}
r(1, 2) &= 1, \quad r(1, 3) = 2, \quad r(1, 4) = 2, \quad r(1, 5) = 3, \quad r(1, 6) = 4, \quad r(1, 7) = 4, \quad r(1, 8) = 4, \quad r(1, 9) = 5, \quad r(1, 10) = 6 \\
r(2, 3) &= 1, \quad r(2, 4) = 1, \quad r(2, 5) = 2, \quad r(2, 6) = 3, \quad r(2, 7) = 3, \quad r(2, 8) = 3, \quad r(2, 9) = 4, \quad r(2, 10) = 5 \\
r(3, 4) &= 2, \quad r(3, 5) = 3, \quad r(3, 6) = 4, \quad r(3, 7) = r(3, 8) = 4, \quad r(3, 9) = 5, \quad r(3, 10) = 6 \\
r(4, 5) &= 1, \quad r(4, 6) = r(4, 7) = r(4, 8) = 2, \quad r(4, 9) = 3, \quad r(4, 10) = 4 \\
r(5, 6) &= r(5, 7) = r(5, 8) = 1, \quad r(5, 9) = 2, \quad r(5, 10) = 3 \\
r(6, 7) &= 2, \quad r(6, 8) = 2, \quad r(6, 9) = 3, \quad r(6, 10) = 4,
\end{align*}
\[ r(7, 8) = 2, \ r(7, 9) = 3, \ r(7, 10) = 4, \]
\[ r(8, 9) = 1, \ r(8, 10) = 2 \]
\[ r(9, 10) = 1 \]

Now, the resistance of molecular graph (G) is equal to the sum of effective resistances between all pairs of vertices of the graph G

\[
R(G) = \sum_{i < j} r(i, j) \\
= (1+2+2+3+4+4+4+5+6) + (1+1+2+3+3+3+4+5) + \\
(2+3+4+4+4+5+6) + (1+2+2+2+3+4) + (1+1+1+2+3) + \\
(2+3+4) + (1+2) + (1) \\
= 127
\]

3.3 PHYSICO - CHEMICAL APPLICATIONS OF THE RESISTANCE OF MOLECULAR GRAPH

The relation between Wiener number W and the boiling points (b. p) of alkanes is given by [4, 9]

\[
b. \ p. = \alpha W + \beta w(3) + \gamma \quad (3.2)
\]

where \( \alpha, \beta \) and \( \gamma \) are empirical constants and \( w(3) \) is the path number, namely, the number of pairs of vertices whose distance is equal to 3. By using this structure property relationship one obtains a reasonable prediction of boiling points of alkanes. It has been observed that Wiener used \( W(G) \) to estimate molar volumes, viscosity, critical pressure, refractive indices, heats of isomerization, heats of vaporization and surface tension of alkanes.
Recently it is shown that the Wiener number measures the extent of branching of the carbon atom skeleton and compactness of given molecule. Wiener number was claimed to be related to intermolecular forces, in case of non-polar molecules like hydrocarbons [10, 11] Correlation between W and melting points were also reported [12, 13]. To some extent, there is a connection between W and the velocity of ultrasound in alkanes and alcohol [8]. The Wiener number finds applications in polymer chemistry. The melting points and other physical properties of polyethylene were predicted on the basis of W-values [14,15]. In studies of crystals, Bonchev [16, 17] put forward a hypothesis that the stability of crystal lattice depends on its Wiener index. Accordingly the configuration whose W is minimal would be most stable one. Based on this hypothesis they characterized the crystal defects in lattice structure.

We claim that, Resistance of the molecular graph \( R(G) \) should have identical applications in various concepts mentioned above as it is identified as equal to W for acyclic molecular structures. Hence the computation of \( R(G) \) for various acyclic molecular structures is of mathematical and physical importance.

### 3.4 EXISTING RESULTS [18, 19, 20]

#### 3.4.1 Wiener index for Linear alkanes with \( n \) carbon atoms

i.e., for path or chain, \( W(P_n) = n(n^2 - 1) / 6 \)  \hspace{1cm} (3.3)

![Fig. 3.3 Path \( P_n \)](image-url)
3.4.2 For star graph with n vertices

\[ W(S_n) = (n - 1)^2 \]  

Fig. 3.4 Star graph \( S_n \)

3.4.3 For comb like branched alkanes with n carbon atoms.

\[ W(\text{Comb}) = \frac{n^3 + 6n^2 - 10n}{12} \]  

Fig. 3.5 Comb - graph

3.4.4 Relation between Wiener numbers of path, tree and star graphs with n vertices is

\[ W(S_n) \leq W(T) \leq W(P_n) \]  

3.4.5 Theorem [21]:

Let \( G \) be a graph with \( n \) vertices and \( e \) edges. Let \( n_1(e) \) and \( n_2(e) = n - n_1(e) \) be the number of vertices of the two components of \( G - e \). Then,

\[ W(G) = \sum_{e} n_1(e) n_2(e) \]  

where the summation goes for all \((n - 1)\) edges.
**Theorem [8] : 3.4.6**

Let $G$ be a tree on $n$ vertices and let $x$ be its branching point, such that the degree of vertex $x$ is $\Delta_x \geq 3$.

Let $n_1, n_2, n_3, \ldots, n_d$ be the number of vertices in the $d$ number of branches attached to vertex $x$ and

$$n_1 + n_2 + n_3 + \ldots + n_d + 1 = n$$

Then

$$W(G) = \left(\frac{n+1}{3}\right) - \sum_{1 \leq i < j < k} n_i n_j n_k$$

(3.8)

**Theorem [22, 23] : 3.4.7**

Let $G$ be a tree with $n$ vertices

then $R(G) = \sum_{i=1}^{n-1} \frac{1}{\lambda_i}$

(3.9)

where $\lambda_1, \lambda_2, \ldots, \lambda_{n-1}, \lambda_n$ are Laplacian eigenvalues of Laplacian matrix which is defined as below.

Let $D$ be the matrix whose diagonal elements are degrees of vertices, viz., $\Delta_1, \Delta_2, \ldots, \Delta_n$ and whose off diagonal elements are equal to zero and let $A$ be the adjacency matrix of the graph then.

$L(G) = (D - A)$ is called the Laplacian matrix of $G$ or Laplacian Polynomial

**3.5 RESULTS**

**Theorem : 3.5.1**

Let $P_n$ be the path with $n$ vertices. Let $B_n$ be the tree with $n$ vertices obtained by branching $P_n$ at end vertex. Then Resistance of $B_n$ is

$$R(B_n) = \frac{1}{6} \left[ n^3 - 7n + 18 \right]$$

(3.10)
Proof:

\[
\begin{align*}
R(B_n) &= R(P_{n-2}) + 2 \left[ r(u_1, u_{n-1}) + r(u_2, u_{n-1}) + \ldots + r(u_{n-2}, u_{n-1}) \right] + r(u_{n-1}, u_n) \\
&= R(P_{n-2}) + 2 \left[ (n-2) + (n-3) + \ldots + 2 + 1 \right] + 2 \\
&= R(P_{n-2}) + 2 \left[ (n+1) - 3 + (n+1) - 4 + (n+1) - 5 + \ldots + (n+1) - (n-1) + (n+1) - n \right] + 2 \\
&= R(P_{n-2}) + 2(n+1)(n-2) - \frac{3+4+5+\ldots+n}{2} + 2 \\
&= R(P_{n-2}) + 2(n+1)(n+2) - n(n+1) + 6 + 2 \\
\end{align*}
\]

From existing result 3.4.1

\[
R(P_n) = \frac{n(n^2-1)}{6}
\]

\[
\Rightarrow R(P_{n-2}) = \frac{(n-2)(n-2)^2 - 1}{6}
\]

\[
= \frac{(n-2)}{6} \left[ n^2 - 4n + 4 - 1 \right]
\]

\[
\therefore R(B_n) = \frac{(n-2)}{6} \left( n^2 - 4n + 3 \right) + 2(n+1)(n-2) - n(n+1) + 6
\]
\[
\begin{align*}
R(B_n) &= \frac{1}{6} \left[ n^3 - 4n^2 + 3n - 2n^2 + 8n - 6 \right] + 2n^2 - 4n + 2n \\
&\quad - 4 - n^2 - n + 8 \\
&= \frac{1}{6} \left[ n^3 - 4n^2 + 3n - 2n^2 + 8n - 6 + 12n^2 - 24n + 12n \right] \\
&\quad - 24 - 6n^2 - 6n + 48 \\
\therefore R(B_n) &= \frac{1}{6} \left[ n^3 - 7n + 18 \right]
\end{align*}
\]

Hence the proof. \[\square\]

**Theorem : 3.5.2**

Let \( R(P_n) \) be the resistance of the path with \( n \) vertices and let \( R(B_n) \) be the resistance of the tree \( B_n \) obtained from \( P_n \), then

\[
R(P_n) - R(B_n) = (n - 3).
\]

**(3.11)**

**Proof :** We have

\[
R(P_n) = \frac{\binom{n+1}{3}}{6} = \frac{n(n^2-1)}{6}
\]

And from our previous theorem,

\[
R(B_n) = \frac{1}{6} (n^3 - 7n + 18)
\]

\[
\therefore R(P_n) - R(B_n) = \frac{1}{6} n(n^2 - 1) - \frac{1}{6} (n^3 - 7n + 18)
\]

\[
= \frac{1}{6} (n^3 - n - n^3 + 7n - 18)
\]

\[
= \frac{1}{6} (6n - 18)
\]
\[ R(P_n) - R(B_n) = (n - 3) \]

**Illustration : 1**  
For \( n = 8 \)

\[
R(P_8) = \frac{n(n^2-1)}{6} = \frac{8(64-1)}{6} = 84
\]

\[
R(B_8) = \frac{1}{6}(n^3 - 7n + 18) = \frac{1}{6}(8^3 - 7 \times 8 + 18) = 79
\]

\[
\therefore R(P_8) - R(B_8) = 84 - 79 = 5
\]

And according to theorem [3.5.2]

\[
R(P_n) - R(B_n) = n - 3 = 5
\]

**Theorem : 3.5.3**

Let \( S_n \) denotes the star graph with \( n \) vertices and let \( A_n \) be the graph obtained from \( S_n \) by removing an edge from star and joining to any pendant vertex of degree one, then \( R(A_n) - R(S_n) = (n - 3) \)  \((3.12)\)

![Graph S_n](image1)

![Graph A_n](image2)

Let \( n \) be the total number of vertices

\[ R(S_n) = (n - 1)^2 \]
In the graph $A_n$, $(n - 1)$ number of vertices form the star graph and $n^{th}$ vertex is pendent vertex.

$$R(A_n) = R(S_{n-1}) + r(v_n, v_{n-1}) + r(v_n, v_{n-2}) + \sum_{j=1}^{n-3} r(v_n, v_j)$$

$$= (n-2)^2 + 1 + 2 + (3 + 3 + \ldots n - 3 \text{ times})$$

$$= n^2 - 4n + 4 + 3 + 3(n - 3)$$

$$= n^2 - n - 2$$

$$R(S_n) - R(A_n) = (n^2 - n - 2) - (n - 1)^2$$

$$= n^2 - n - 2 - n^2 + 2n - 1$$

$$= n - 3$$

For example: Consider $n = 8$,

$$R(S_8) = (n - 1)^2 = (8 - 1)^2 = 49$$

$$R(A_8) = n^2 - n - 2 = 64 - 8 - 2 = 54$$

$$R(A_8) - R(S_8) = 54 - 49 = 5.$$  

Also, $(n - 3) = 5$.

Hence the theorem.

Lemma : 3.5.4

There does not exist integral triplets \{x, y, z\} and \{a, b, c,\} satisfying the equations

$$x + y + z = a + b + c$$

$$xyz = abc \quad \text{Simultaneously}$$

Proof : If $(x, y, z) \neq (a, b, c)$ then the following are the possibilities

i) $x = a, \ y = b, \ z \neq c$  or  ii) $x = a, \ y \neq b, \ z = c$

iii) $x \neq a, \ y = b, \ z = c$  or  iv) $x = a, \ y \neq b, \ z \neq c$

70
Consider the following condition

Let \( x = a \) and \( y \neq b, \ z \neq c \)

\[
\begin{align*}
\{ x + y + z &= a + b + c \\
x y z &= a b c \\
y + z &= b + c \quad \text{and} \\
y z &= b c
\}
\]

becomes

\[
(3.13)
\]

\[
(3.14)
\]

Squaring (3.13)

\[
(y + z)^2 = (b + c)^2
\]

Substract 4 \( yz \) from both side

\[
(y + z)^2 - 4 yz = (b + c)^2 - 4 bc
\]

\[
\Rightarrow (y - z)^2 = (b - c)^2
\]

\[
\Rightarrow (y - z) = \pm (b - c)
\]

\[
\Rightarrow (y - z) = (c - b) \quad (3.15)
\]

\[
\text{OR} \quad (y - z) = (b - c) \quad (3.16)
\]

From (3.13) and (3.15) we get

\[
y = c \quad \text{and} \quad z = b
\]

From (3.13) and (3.16) we get

\[
y = b \quad \text{and} \quad z = c
\]

which is a contradiction to the assumption

that \( y \neq b \) and \( z \neq c \)

The proof is similar in rest of the above conditions

Hence the lemma.
Theorem: 3.5.5

No two trees of same order with exactly one vertex of degree 3 and others are of degree ≤ 2 have same resistance.

Proof:

Let \( T_1 \) and \( T_2 \) be two trees each with \( n \) vertices. Let \( u \) and \( v \) be the vertices of degree 3 in \( T_1 \) and \( T_2 \) respectively. Let \( T_1 - u \) has exactly 3 components of order \( x, y, \) and \( z \) and \( T_2 - v \) has 3 components of orders \( a, b, \) and \( c \) respectively.

Then, by the theorem [3.4.6] we have.

\[
R(T_1) = \binom{n+1}{3} - xyz
\]

\[
R(T_2) = \binom{n+1}{3} - abc
\]

Now we claim that, the sum over the resistances distance between all pairs of vertices of trees \( T_1 \) and \( T_2 \) are not equal.

i.e., \( R(T_1) \neq R(T_2) \)

For if, \( R(T_1) = R(T_2) \) then

\[
xyz = abc
\]

Also, since \( T_1 \) and \( T_2 \) are of the same order

\[
x + y + z = a + b + c = (n - 1)
\]

But, by the lemma (3.5.4) the equations, viz.,

\[
xyz = abc
\]

and \( x + y + z = a + b + c \)

have no integral solutions

\[
\therefore R(T_1) = R(T_2) \text{ does not holds}
\]

Hence the claim.
3.6 COMPUTATION OF $R(G)$ FOR MOLECULAR GRAPHS.

We consider the following two examples of molecular graphs and apply various methods of computing the resistance distance.

3.6.1 Wiener method [9] Originally this method was used to compute the Wiener index for tree. Similarly, resistance of the molecular graph could be obtained by summing the products of number of carbon bonds on one side of any bond by those on the other side. Let $T$ be a tree with $n$ vertices, and $e$ one of its edges. Let $n_1(e)$ and $n_2(e) = n - n_1(e)$ be the number of vertices on the two parts of $T - e$. Then,

$$R(G) = \sum_{e} n_1(e) n_2(e)$$

Summation goes over $(n - 1)$ edges

Referring to above Figure (3.10) we see that $G - e_1$ leaves two components one with one vertex and other with 13 vertices.
Similarly $G - e_2$ leaves two components so that
\[ \Rightarrow n_1(e_2) n_2(e_2) = 1 \times 13 = 13 \]
And so on we have,
\[ n_1(e_3) n_2(e_3) = 3 \times 11 = 33 \]
\[ n_1(e_4) n_2(e_4) = 4 \times 10 = 40 \]
\[ n_1(e_5) n_2(e_5) = 5 \times 9 = 45 \]
\[ n_1(e_6) n_2(e_6) = 2 \times 12 = 24 \]
\[ n_1(e_7) n_2(e_7) = 1 \times 13 = 13 \]
\[ n_1(e_8) n_2(e_8) = 8 \times 6 = 48 \]
\[ n_1(e_9) n_2(e_9) = 3 \times 11 = 33 \]
\[ n_1(e_{10}) n_2(e_{10}) = 1 \times 13 = 13 \]
\[ n_1(e_{11}) n_2(e_{11}) = 1 \times 13 = 13 \]
\[ n_1(e_{12}) n_2(e_{12}) = 2 \times 12 = 24 \]
\[ n_1(e_{13}) n_2(e_{13}) = 1 \times 13 = 13 \]
\[
R(G) = \sum_{e} n_1(e) n_2(e) = 325
\]
Use of this method for the second molecular graph, viz., 2, 3, 4- trimethyl 3-ethylheane will give us the resistance
\[
R(G) = 148
\]

3.6.2 Method based on the concept of branching of vertices (8).

If the number of vertices in the branches attached to vertex $x$ are denoted by $n_1, n_2, \ldots n_d$, for $d$ number of branches

Then,
\[
R(G) = \left( \frac{n+1}{3} \right) - \sum_{x} \sum_{i < j < k} n_i n_j n_k
\]

74
Consider the Figure 3.10 representing the molecular graph of 5 ethyl - 6 - isoproply - 2 methyloctane. \( n = 14 \)

\[
\text{Now } \binom{n+1}{3} = \frac{15 \times 14 \times 13}{3 \times 2} = 455
\]

Let us calculate the second term on R.H.S. at each branching vertex.

At vertex 2, \( n_1 n_j n_k = 1 \times 1 \times 11 = 11 \)

At vertex 6, \( n_1 n_j n_k = 5 \times 2 \times 6 = 60 \)

At vertex 9, \( n_1 n_j n_k = 8 \times 3 \times 2 = 48 \)

At vertex 10, \( n_1 n_j n_k = 11 \times 1 \times 1 = 11 \)

\[
\therefore R(G) = 455 - (11 + 60 + 48 + 11) = 325
\]

Let us consider the other example of Figure 3.11. It is redrawn as in Figure 3.12.

Molecular Graph of 2, 3, 4 - trimethyl - 3 ethyl hexane.

\[
\binom{n+1}{3} = \frac{12 \times 11 \times 10}{3 \times 2} = 220
\]

Consider branching point \( x_1 \)

\( n_1 n_j n_k = 1 \times 1 \times 8 = 8 \)

The branching point \( x_2 \) has 4 branches with 3, 1, 2 and 4 vertices.
\[ \sum_{i < j < k} n_i n_j n_k = 1 \times 2 \times 3 + 2 \times 3 \times 4 + 3 \times 4 \times 5 + 4 \times 1 \times 2 = 50 \]

Now, at the branching point \( x_3 \),
\[ n_i n_j n_k = 7 \times 1 \times 2 = 14 \]
\[ \sum \sum n_i n_j n_k = 8 + 50 + 14 = 72 \]
\[ R(G) = \left( \frac{n+1}{3} \right) - \sum \sum n_i n_j n_k = 220 - 72 = 148. \]

3.6.3 Use of resistance distance matrix

In this method we compute the effective resistance between every pair of vertices of molecular graph and put them in the form of matrix, which is symmetric of order \( n \times n \). Following matrix shows the resistance matrix for the example referred in Figure 3.10 of molecular graph of 5-ethyl-6-isopropyl-2-methyloctane.

\[
\begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 \\
1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 2 & 5 & 6 & 6 & 7 & 7 \\
2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 1 & 4 & 5 & 5 & 6 & 6 \\
3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 2 & 3 & 4 & 4 & 5 & 5 \\
4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 3 & 3 & 4 & 4 \\
5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 1 & 2 & 2 & 3 & 3 \\
6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 5 & 2 & 3 & 1 & 2 & 2 \\
7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 6 & 3 & 4 & 2 & 3 & 3 \\
8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 7 & 4 & 5 & 3 & 4 & 4 \\
9 & 2 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 0 & 5 & 6 & 6 & 7 & 7 \\
10 & 5 & 4 & 3 & 2 & 1 & 2 & 3 & 4 & 5 & 0 & 1 & 3 & 4 & 4 \\
11 & 6 & 5 & 4 & 3 & 2 & 3 & 4 & 5 & 6 & 1 & 0 & 4 & 5 & 5 \\
12 & 6 & 5 & 4 & 3 & 2 & 1 & 2 & 3 & 6 & 3 & 4 & 0 & 1 & 1 \\
13 & 7 & 6 & 5 & 4 & 3 & 2 & 3 & 4 & 7 & 4 & 5 & 1 & 0 & 2 \\
14 & 7 & 6 & 5 & 4 & 3 & 2 & 3 & 4 & 7 & 4 & 5 & 1 & 2 & 0
\end{bmatrix}
\]
By definition

\[ R(G) = \frac{1}{2} \text{ sum of the elements of } RD \text{ matrix} \]

\[ = \frac{1}{2} \times 650 = 325 \]

3.6.4 Use of Laplacian eigen values in computing the resistance of graph.

Fig. 3.13 Graph G : P₃

Consider a simple path with \( n = 3 \) vertices. The adjacency matrix \( A \) is

\[
A(G) = \begin{bmatrix}
0 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0
\end{bmatrix}
\]

The degree matrix \( D \) is

\[
D(G) = \begin{bmatrix}
1 & 0 & 0 \\
0 & 2 & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

\[ \therefore \text{ Laplacian matrix of graph } G \]

\[
L(G) = D(G) - A(G)
\]

\[
= \begin{bmatrix}
1 & -1 & 0 \\
-1 & 2 & -1 \\
0 & -1 & 1
\end{bmatrix}
\]

The characteristic equation is of the form

\[ L - \lambda I = 0 \]

where \( I \) is the identity matrix

The laplacian eigenvalues are obtained by solving the equation
in the matrix form.

\[
\begin{bmatrix}
1 - \lambda & -1 & 0 \\
-1 & 2 - \lambda & -1 \\
0 & -1 & 1 - \lambda
\end{bmatrix} = 0
\]

\[
\Rightarrow (1 - \lambda) [(-2 + \lambda)(1 - \lambda) - 1] - (-1) [-1 (1 - \lambda)] + 0 = 0
\]

\[
\Rightarrow (1 - \lambda)(\lambda^2 - 3\lambda + 1) - (1 - \lambda) = 0
\]

\[
\Rightarrow \lambda = 1, \quad \lambda = 0, \quad \lambda = 3
\]

i.e., Laplacian eigen values are

\[
\lambda_1 = 0, \quad \lambda_2 = 1, \quad \lambda_3 = 3.
\]

By the existing result [4.4.7]

\[
R(G) = n \sum_{i=1}^{n} \frac{1}{\lambda_i} = 3 \left[1 + \frac{1}{3}\right]
\]

\[
\therefore R(G) = 4
\]

### 3.7 Co-Resistance Molecular Structures

In case of trees the resistance matrix is equivalent to the distance matrix which records the length of the shortest path between vertices and the sum of the matrix elements above the diagonal gives the topological index under study i.e., the resistance of the structure. In correlation with several other topological indices this resistance could be tested for boiling points of alkanes and cycloalkanes.

It is well known that, topological indices show degeneracy [24] that is, two or more non-isomorphic graphs may have identical numerical values for an index. We have computed resistance distances for all possible tree graphs with vertices \(n = 4, 5, 6, 7\)
and 8. We observed that following pairs of tree graphs shows degeneracy property and we call them as co-resistance molecular structures.

Fig. 3.14 Two pairs of trees with \( n = 7 \), having same Resistance

Fig. 3.15 Three pairs of trees with \( n = 8 \), having same resistance
It is interesting to see that this degeneracy occurs sometimes for small graphs and sometimes for graphs of intermediate size. The resistance $R(G)$, a graph invariant, could be used to find the size of the smallest graphs that show the property of degeneracy. This property of invariants is observed to be helpful in differentiating structural variations among similar compounds.

Figure 3.14 and Figure 3.15 represent the smallest graphs in pairs that show the property of degeneracy. For $n = 7$ (the number of vertices) we have two pairs of trees one with Resistance 48 and other with 46

\[ R(G_1) = R(G_2) = 48 \]
\[ R(G_3) = R(G_4) = 46 \]

For $n = 8$, we have 3 pairs of trees having identical resistance viz.,

\[ R(G_1) = R(G_2) = 71 \]
\[ R(G_3) = R(G_4) = 67 \]

And \[ R(G_5) = R(G_6) = 62 \]

Though the pair of graphs have the same resistance value, the elements of their resistance matrices are different and their structures are also different. For example consider the following.

\[
\begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 \\
0 & 1 & 2 & 3 & 4 & 4 & 4 \\
1 & 0 & 1 & 1 & 2 & 3 & 3 \\
2 & 1 & 0 & 2 & 3 & 4 & 4 \\
2 & 1 & 2 & 0 & 1 & 2 & 2 \\
3 & 2 & 3 & 1 & 0 & 1 & 1 \\
4 & 3 & 4 & 2 & 1 & 0 & 2 \\
4 & 3 & 4 & 2 & 1 & 2 & 0 \\
\end{bmatrix}
\]

RD matrix of 2-4, dimethylpentane \[ R(G_1) = 48 \]

\[
\begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 \\
1 & 0 & 1 & 2 & 3 & 3 & 3 \\
2 & 1 & 0 & 1 & 2 & 1 & 2 \\
3 & 2 & 1 & 0 & 1 & 2 & 3 \\
4 & 3 & 2 & 1 & 0 & 3 & 4 \\
3 & 2 & 1 & 2 & 3 & 0 & 1 \\
4 & 3 & 2 & 3 & 4 & 1 & 0 \\
\end{bmatrix}
\]

RD matrix of 3 ethylepentane \[ R(G_2) = 48 \]

80
The occurrence of identical index \( R(G) \) for non-isomorphic graph represents an interesting situation.

Mean isomer degeneracy [8, 25 - 28] is defined as

\[
\mu = \frac{N}{t}
\]

where \( N \) is the number of distinct structural isomers and \( t \) is the number of distinct value of resistance assumes for these isomers.

\( \mu = 1 \), if \( R \) are different

\( \mu > 1 \), if \( R \) is same

For example if \( n = 4, 5, 6 \) Each tree graph has different value of resistance i.e., \( R(G) \) are distinct. Therefore

\( \mu = 1 \)

Consider the same case of isomeric alkanes for \( n = 7 \), there are 9 structural isomers (i.e., total number of trees except path and star) But they have only 7 distinct values of \( R \)

\[
\therefore \mu = \frac{9}{7} = 1.29 > 1
\]

It is observed that [29] the mean isomer degeneracy increases as \( n \) increases.
The following figures represent the acyclic trees (Molecular Structures) of \( n = 4 \) to \( n = 8 \) vertices. The chemical names and the resistance of the chemical structure are indicated immediately below each tree graph.

\[
\begin{align*}
\text{butane} & \quad R(G) = 10 \\
2\text{-methly propane} & \quad R(G) = 9
\end{align*}
\]

Fig. 3.16 **Two** tree graphs with \( n = 4 \) vertices

\[
\begin{align*}
pentane & \quad R(G) = 20 \\
2\text{-methyle butane} & \quad R(G) = 18 \\
2,2 \text{ dimethyl propane} & \quad R(G) = 16
\end{align*}
\]

Fig. 3.17 **Three** tree graphs with \( n = 5 \) vertices

\[
\begin{align*}
hexane & \quad R(G) = 35 \\
2\text{-methyl pentane} & \quad R(G) = 32
\end{align*}
\]

\[
\begin{align*}
2,3\text{-dimethyl butane} & \quad R(G) = 31 \\
2, 2 \text{ dimethyl butane} & \quad R(G) = 29
\end{align*}
\]

\[
\begin{align*}
2,2\text{-dimethyl butane} & \quad R(G) = 28 \\
\text{} & \quad R(G) = 25
\end{align*}
\]

Fig. 3.18 **Six** tree graphs with \( n = 6 \) vertices.
Fig. 3.19 Eleven tree graphs with $n = 7$ vertices
Fig. 3.20 Fourteen of the Twenty Three tree graphs with \( n = 8 \)
Fig. 3.20 Remaining Nine of Twenty three tree graphs with $n = 8$ vertices
REFERENCES


2. F. Buckley and F. Harary, *Distance in Graphs* [Addison-Wesley, Reading, (1989)]


7. A. Cayley, Philos Mag. (1874), 47, 444.


