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Randic index of various classes of graphs formed on the basis of some graph combinations

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***Abstract**: The Randic index R(G) of a graph G=(V,E) is defined as follows* $R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}}$
Here d_u and d_v are the degrees of vertices u and v respectively. In this paper, we give explicit computing formulae for various classes of graphs formed on the basis of two types of Combinations A and B. Moreover, we introduce a relationship between the randic index of combined graphs G_A ,G_B and first Zagreb index.
***Keywords**: Randic index, degree of a vertex, edge, path graph P_n , first Zagreb index.*

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I. INTRODUCTION

Molecular descriptors play a fundamental role in chemistry, quality control, pharmaceutical sciences, environmental protection policy and health researches; allowing some mathematical treatment of the chemical information contained in the molecule. This was defined by Todeschini and Consonni as [9]:

"The molecular descriptor is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment."

By this definition, the molecular descriptors are divided into two main categories: experimental measurements, such as log P, molar refractivity, dipole moment, polarizability, and, in general, physico-chemical properties, and theoretical molecular descriptors, which are derived from a symbolic representation of the molecule and can be further classified according to the different types of molecular representation.

The main classes of theoretical molecular descriptors are: 0D-descriptors (i.e. constitutional descriptors, count descriptors), 1D-descriptors (i.e. list of structural fragments, fingerprints), 2D-descriptors (i.e. graph invariants), 3D-descriptors (such as, for example, 3D-MoRSE descriptors, WHIM descriptors, GETAWAY descriptors, quantum-chemical descriptors, size, steric, surface and volume descriptors), 4D-descriptors (such as those derived from GRID or CoMFA methods, Volsurf).

We are interested to discuss one kind of 2D-descriptor, graph invariants.

In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Its vertices are labeled with the kinds of the corresponding atoms and edges are labeled with the types of bonds.

Arthur Cayley[1] was probably the first to publish results that consider molecular graphs as early as in 1874, even before the introduction of the term "graph". For the purposes of enumeration of isomers, Cayley considered "diagrams" made of points labelled by atoms and connected by links into an assemblage.

A graph G consists of a finite non empty set V=V(G) of m points together with a prescribed set E(G) of n unordered pairs of distinct points of V. The sets, V is called as vertex set and E = E(G) is known as the edge set of G.

When we study the abstract structure of graphs, a graph property is defined to be a property preserved under all possible isomorphisms of a graph. In other words, it is a property of the graph itself, not of a specific drawing or representation of the graph. Informally, the term "graph invariant" is used for properties expressed quantitatively, while "property" usually refers to descriptive characterizations of graphs. For example, the statement "graph does not have vertices of degree 1" is a "property" while the number of vertices of degree 1 in a graph" is an "invariant".

Topological indices are numerical parameters of graph invariants. There are several type of topological indices like wiener index, Hosoya index, Zagreb Index etc.

In 1975, the chemist Milan Randic [7] proposed a topological index R under the name "branching index", suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The branching index was renamed the molecular connectivity index and is often referred to as the Randic index.

There is a good correlation between the Randic index and several physic-chemical properties of alkanes: boiling points, enthalpies of formation, chromatographic retention times, etc. [2],[4],[5].

The Randic index R(G) of a graph G=(V,E) is defined as follows

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}}$$

Here d_u and d_v are the degrees of vertices u and v respectively.

II. PRELIMINARIES

In this section first we recall the definitions of various classes of graphs.

Definition 2.1: Path graph is a graph whose vertices can be arranged in the order $v_1, v_2, \ldots\ldots, v_{n,} v_{n+1}$ such that the edges are $\{v_i, v_{i+1}\}$ where i = 1, 2, …., n. A path of length n is denoted by P_n.

Definition 2.2: The star graph S_n is a graph consisting of n vertices with one central vertex having degree n-1 and the other n-1 vertices having degree 1.

Definition 2.3: If every vertex of a graph has degree 2, then the graph is said to be Cyclic Graph. The number of edges in a cycle is the length of the cycle. A Cycle of length n is denoted by C_n.

Now, we discuss two types of graph Combinations.

Definition 2.4: Combination A: Suppose that G is a nontrivial connected graph and v be any arbitrary vertex in G. The combined graph G_A based on Combination A is obtained from G by attaching at v two paths P : $vu_1u_2 \ldots u_k$ of length k and Q : $vw_1w_2 \ldots w_l$ of length l.

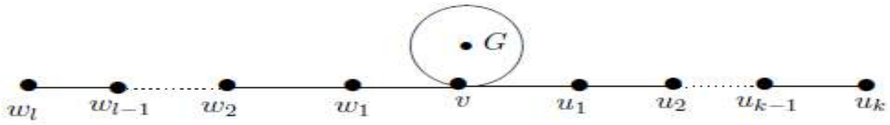

Fig 1: G_A - Combination A

Definition 2.5. *Combination B: Suppose that G is a nontrivial connected graph and v be any arbitrary vertex in G.The combined graph G_B based on Combination B is obtained from G by attaching a path of length k+l at v.* $G_B = G_A - vw_1 + u_kw_1$

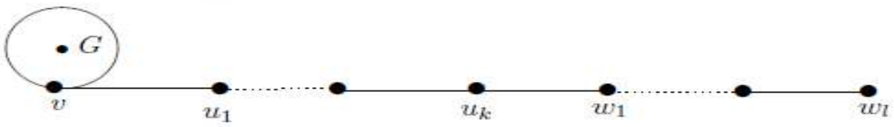

Fig 2: G_B - Combination B

Definition 2.6. *[6] The first general Zagreb index $M_1^\alpha(G)$ is defined as*

$$M_1^\alpha(G) = \sum_{v \in V} d(v)^\alpha$$

where α is any real number except 0 and 1.

III. PREVIOUS RESULTS

3.1 Randic index of Path graph, P_n [8]

$R(P_1) = 0$

$R(P_2) = 1$

For $n \geq 3$,

Let $v_1, v_2, \ldots\ldots, v_{n+1}$ be a path graph P_n consisting of n+1 vertices and n edges.

The vertices v_1 and v_{n+1} are pendent vertices and all other vertices are of degree 2. So the Randic index contribution of first and last edge is $\sqrt{2}$.
Out of the remaining n-2 edges, both the end vertices are of degree 2.
Hence the Randic index of Path graph, P_n is

$$R(P_n) = \sqrt{2} + \frac{n-2}{2}$$

3.2 Randic index of Star graph, S_n[8]

Let $vv_1v_2\cdots v_{n-1}$ be a star graph S_n containing n vertices and $n-1$ edges. Let v be the central vertex of S_n. All of these n-1 edges have pendent vertices and dominating vertices. Hence the Randic index of Star graph, S_n is

$$R(S_n) = \frac{n-1}{\sqrt{n-1}} = \sqrt{n-1}$$

IV. MAIN RESULTS

First we focus to find the randic index of combined graphs of three well known graphs with respect to the Combination A

4.1 Randic index of combined graph G_A of path graph P_n

Case 1: We assume one of P_n, P_l, P_k is a path of length 1.

Table 1:

cases	length of P_n	length of P_l	length of P_k	Randic index of combined graph G_A is
a	1	1	1	$\sqrt{3}$.
b	1	1	$k>1$	$\sqrt{2}+\frac{k-2}{2}-\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}+\frac{2}{\sqrt{3}}$.
c	1	$l>1$	1	$\sqrt{2}+\frac{l-2}{2}-\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}+\frac{2}{\sqrt{3}}$.
d	$n>1$	1	1	$\sqrt{2}+\frac{n-2}{2}-\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}+\frac{2}{\sqrt{3}}$,if we attach P_l and P_k at $\{v_1, v_{n+1}\}$ of P_n. $\sqrt{2}+\frac{n}{2}-\frac{1}{\sqrt{2}}+\frac{1}{2\sqrt{2}}$,if we attach P_l and P_k at $\{v_2, v_n\}$ of P_n. $\sqrt{2}+\frac{n}{2}-1+\frac{1}{\sqrt{2}}$,if we attach P_l and P_k at $v_3, v_4, \cdots, v_{n-1}$ of P_n.
e	1	$l>1$	$k>1$	$\frac{l+k}{2}-2+\sqrt{2}+\frac{\sqrt{2}+1}{\sqrt{3}}$.
f	$n>1$	1	$k>1$	$\frac{n+k}{2}-2+\sqrt{2}+\frac{\sqrt{2}+1}{\sqrt{3}}$,if we attach P_l and P_k at $\{v_1, v_{n+1}\}$ of P_n. $\frac{n+k-3}{2}+\sqrt{2}+\frac{1}{\sqrt{2}}$,if we attach P_l and P_k at $\{v_2, v_n\}$ of P_n. $\frac{n+k-4}{2}+2\sqrt{2}-\frac{1}{2}+\frac{1}{2\sqrt{2}}$, if we attach P_l and P_k at $\{v_3, v_4, \cdots, v_{n-1}\}$ of P_n.
g	$n>1$	$l>1$	1	$\frac{n+l}{2}-2+\sqrt{2}+\frac{\sqrt{2}+1}{\sqrt{3}}$,if we attach P_l and P_k at $\{v_1, v_{n+1}\}$ of P_n. $\frac{n+l-3}{2}+\sqrt{2}+\frac{1}{\sqrt{2}}$,if we attach P_l and P_k at $\{v_2, v_n\}$ of P_n. $\frac{n+l-4}{2}+2\sqrt{2}-\frac{1}{2}+\frac{1}{2\sqrt{2}}$, if we attach P_l and P_k at $\{v_3, v_4, \cdots, v_{n-1}\}$ of P_n.

Now, we assume all of P_n, P_l, P_k are path graphs of length > 1.
Case 2: Suppose G_A is obtained by attaching P_l and P_k at pendent vertices $\{v_1, v_{n+1}\}$ of P_n:

The combined graph G_A is refered by

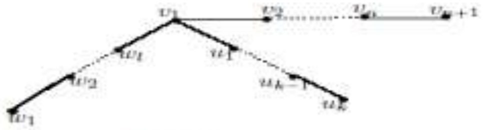

Fig 3: G_A

We have, the Randic index of Path graph P_n is $R(P_n) = \sqrt{2} + \frac{n-2}{2}$
Hence, the Randic contribution of $n+l$ edges is $R(P_{n+1}) - 1 + \frac{1}{\sqrt{6}}$
The Randic index contribution of remaining k edges is $\sqrt{2} + \frac{k-2}{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}}$
Therefore, the Randic index of G_A is

$$\begin{aligned} R(G_A) &= R(P_{n+l}) - 1 + \frac{1}{\sqrt{6}} + \sqrt{2} + \frac{k-2}{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} \\ &= \frac{n+l+k}{2} - 3 + 2\sqrt{2} + \frac{\sqrt{3}-1}{\sqrt{2}} \end{aligned}$$

Case 3: Suppose G_A is obtained by attaching P_l and P_k at vertices $\{v_2, v_n\}$ of P_n:
The combined graph G_A is refered by

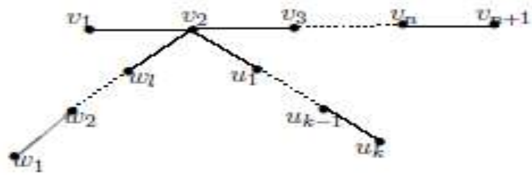

Fig 4: G_A

The Randic index contributions of edges of P_n is $R(P_n) - \frac{1}{\sqrt{2}} + \frac{1}{2\sqrt{2}}$
Also, the Randic index contribution of remaining l+k edges is
$R(P_l) - \frac{1}{\sqrt{2}} + \frac{1}{2\sqrt{2}} + R(P_k) - \frac{1}{\sqrt{2}} + \frac{1}{2\sqrt{2}}$

Hence, Randic index of G_A is

$$R(G_A) = \frac{n+l+k-6}{2} + 3\sqrt{2} - \frac{3}{\sqrt{2}} + \frac{3}{2\sqrt{2}}$$

Case 4: Suppose G_A is obtained by attaching P_l and P_k at $\{v_3, v_4, \cdots, v_{n-1}\}$ of P_n.
The combined graph G_A is refered by

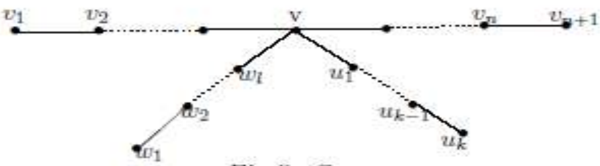

Fig 5: G_A

The Randic index contributions of edges of P_n is $R(P_n) - 1 + \frac{1}{\sqrt{2}}$
The Randic index contributions of edges of P_l is $R(P_l) + \frac{1}{\sqrt{2}}$
Similarly, Randic index contributions of remaining k edges is $R(P_k) + \frac{1}{\sqrt{2}}$
Combining all these contributions, Randic index of G_A is

$$R(G_A) = \frac{n+l+k}{2} + \frac{3}{\sqrt{2}} + 3\sqrt{2} - 4$$

4.2 Randic index of combined graph G_A of star graph $S_n, \geq 2$

Case 1: Let the length of one of P_l,P_k is a path of length 1.

cases	length of P_l	length of P_k	Randic index of combined graph $R_{(G_A)}$ is
a	1	1	$n+1$,if we attach P_l and P_k at central vertex of S_n. $\frac{n-2}{\sqrt{n-1}} + \frac{1}{\sqrt{3(n-1)}} + \frac{2}{\sqrt{3}}$,if we attach P_l and P_k at one pendent vertex of S_n.
b	1	$k > 1$	$\sqrt{n+1} + \frac{k-2}{2} + \sqrt{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(n+1)}}$,if we attach P_l and P_k at central vertex of S_n. $\frac{n-2}{\sqrt{n-1}} + \frac{1}{\sqrt{3(n-1)}} + \frac{1}{\sqrt{3}} + \frac{k-2}{2} + \sqrt{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}}$,if we attach P_l and P_k at one pendent vertex of S_n.
c	$l > 1$	1	$\sqrt{n+1} + \frac{l-2}{2} + \sqrt{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(n+1)}}$,if we attach P_l and P_k at central vertex of S_n. $\frac{n-2}{\sqrt{n-1}} + \frac{1}{\sqrt{3(n-1)}} + \frac{1}{\sqrt{3}} + \frac{l-2}{2} + \sqrt{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}}$,if we attach P_l and P_k at one pendent vertex of S_n.

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Table 2:

Now,we assume both P_l,P_k are path graphs of length > 1.

Case 2: Suppose G_A is obtained by attaching P_l and P_k at central vertex of S_n:

The calculation of Randic index of G_A is divided into,

- With respect to the edges of S_n.
- With respect to the edges of P_l.
- With respect to the edges of P_k.

S_n contribute n-1 edges and the degree of the incident vertices of all these edges are 1 and $n+1$.

The randic index contribution with respect to the edges of S_n is

$$\frac{n-1}{\sqrt{n+1}} \tag{4.1}$$

The randic index contribution of P_l is

$$R(P_l) = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(n+1)}} \tag{4.2}$$

The randic index contribution of P_k is

$$R(P_k) = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(n+1)}} \tag{4.3}$$

Adding equations 4.1,4.2 and 4.3
The Randic index of G_A is $\frac{n-1}{\sqrt{n+1}} + \frac{l+k-4}{2} + \sqrt{2} + \frac{\sqrt{2}}{n+1}$

Case 3: Suppose G_A is obtained by attaching P_l and P_k at one pendent vertex of S_n:

The graph structure of G_A is described by the following table.

Number of edges	Degree of incident vertices
n-2	(1,n-1)
1	(3,n-1)
l+k-4	(2,2)
2	(1,2)
2	(2,3)

Therefore, The randic index of G_A is

$$\frac{n-2}{\sqrt{n-1}} + \frac{1}{\sqrt{3(n-1)}} + \frac{l+k-4}{2} + \sqrt{2} + \frac{2}{\sqrt{6}}$$

4.3 Randic index of combined graph G_A of cyclic graph $C_n, \forall n \geq 2$

Case 1:Length of one of path graphs P_l,P_k is 1.

cases	length of P_l	length of P_k	Randic index of combined graph $R(G_A)$ is
a	1	1	$\frac{n-2}{2} + \frac{1}{\sqrt{2}} + 1.$
b	1	$k > 1$	$\frac{n+k-4}{2} + \frac{1}{2} + \sqrt{2} + \frac{1}{2\sqrt{2}}$
c	$l > 1$	1	$\frac{n+l-4}{2} + \frac{1}{2} + \sqrt{2} + \frac{1}{2\sqrt{2}}$

Table 4:

Case 2:Assume both P_l,P_k are path graphs of length greater than 1.
Let G be acyclic graph with n vertices.Attach P_l,P_k at any vertex of G.Let that vertex be v.
The vertices $V(G) \setminus \{v\}$ contribute n-2 edges whose incident vertices are of degree 2.The 2 edges meets with v contribute the randic index contribution of $\frac{1}{\sqrt{2}}$.The newly attached P_l,P_k contribute $l+k$ edges .These $l+k$ edges are described by the following table.

Number of edges	Degree of incident vertices
2	(1,2)
2	(2,4)
l+k-4	(2,2)

So, The randic index contribution of these l+k edges is $\sqrt{2} + \frac{1}{\sqrt{2}} + \frac{l+k-4}{2}$.
Summing up all edge contributions,the randic index of G_A is

$$R(G_A) = \frac{n-2}{2} + \frac{l+k-4}{2} + 2\sqrt{2}$$

4.4 General formula for the Randic index of combined graph G_A of a connected graph G

Assume that both P_l,P_k are path graphs of length greater than 1.

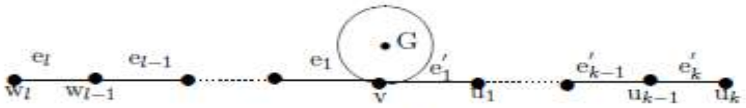

Fig 6: G_A - Combination A of G

Suppose we attach P_l and P_k at a vertex v of G.Let the degree of v be m.Let $y_1, y_2, \cdots, y_m$ be the degree of the vertices in the neighbour set of v.
First, we will find the randic contribution of P_l :
The edge set of P_l is $E_1 = \{e_1, e_2, \cdots, e_{l-1}, e_l\}$.All the edges of $E_1 \setminus \{e_1, e_l\}$ incident the vertices of degree 2. The one end of last edge e_l is pendent vertex and the other end meets with a vertex of degree 2.The end vertices of first edge (e_1 ie,the connecting edge of P_l with G) are of degree 2 and $m+2$.
Similarly,We can calculate the Randic index contributions of the edge set$E_2 = \{e'_1, e'_2, \cdots, e'_{k-1}, e'_k\}$ of P_k.
Summing up all these, the randic index contributions of the edges in $E_1 \cup E_2$ is

$$\frac{l+k-4}{2} + \sqrt{2} + \frac{\sqrt{2}}{\sqrt{m+2}} \tag{4.4}$$

By the combination of A, Randic index contribution of edges in G changes to

$$R(G) - \sum_{i=1}^{m} \frac{1}{\sqrt{y_i m}} + \sum_{i=1}^{m} \frac{1}{\sqrt{y_i(m+2)}} \tag{4.5}$$

Adding equations 4.4 and 4.5,
The randic index of combined graph G_A of a connected graph G is

$$R_A(G) = R(G) + \frac{l+k-4}{2} + \sqrt{2} + \frac{\sqrt{2}}{\sqrt{m+2}} - \sum_{i=1}^{m} \frac{1}{\sqrt{y_i m}} + \sum_{i=1}^{m} \frac{1}{\sqrt{y_i(m+2)}} \tag{4.6}$$

4.5 General formula for the Randic index of combined graph G_B of a connected graph G

Suppose we attach a path of length $l+k$ (where $l+k \geq 2$) at a vertex v of G during the construction of G_B.

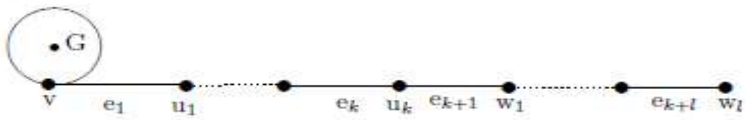

Fig 7: G_B - Combination B of G

Let the degree of v be m. Let$y_1, y_2, \cdots, y_m$ be the degree of the vertices in the neighbour set of v.
Let the edge set of P_{k+l} is $E = \{e_1, e_2, \cdots, e_{k-1}, e_k, e_{k+1}, \cdots, e_{k+l}\}$.
All the edges of $E \setminus \{e_1, e_{k+l}\}$ meets its ends at vertices of degree 2. The one end of e_{k+l} is pendent vertex and the other vertex of degree 2.The end vertices of e_1 are of degree $m+1$ and 2.
So,the Randic index contributions of the edges in E is

$$\frac{l+k-2}{2} + \sqrt{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(m+1)}} \tag{4.7}$$

By the combination B, Randic index contribution of edges in G changes to

$$R(G) - \sum_{i=1}^{m} \frac{1}{\sqrt{y_i m}} + \sum_{i=1}^{m} \frac{1}{\sqrt{y_i(m+1)}} \tag{4.8}$$

Adding equations 4.7 and 4.8,
The randic index of combined graph G_B of a connected graph G is

$$R_B(G) = R(G) + \frac{l+k-2}{2} + \sqrt{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(m+1)}} - \sum_{i=1}^{m} \frac{1}{\sqrt{y_i m}} + \sum_{i=1}^{m} \frac{1}{\sqrt{y_i(m+1)}} \tag{4.9}$$

4.6 Relationship between Randic index of combined graphs G_A and G_B of a connected graph G with first general Zagreb index

From 4.6 and 4.9,
$R_A(G) - R_B(G)$

$$= \frac{1-\sqrt{2}}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{m+2}} - \frac{1}{\sqrt{2(m+1)}} + \sum_{i=1}^{m} \frac{1}{\sqrt{y_i(m+2)}} - \sum_{i=1}^{m} \frac{1}{\sqrt{y_i(m+1)}}$$
$$= \sum_{i=1}^{m} \frac{1}{\sqrt{y_i}}[\frac{1}{\sqrt{m+2}} - \frac{1}{\sqrt{m+1}}] + \frac{1-\sqrt{2}}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{m+2}} - \frac{1}{\sqrt{2(m+1)}} \quad (4.11)$$

Let $U = \{v_1, v_2, \cdots, v_m\}$ be the neighbour set of vertex v and W be the edges $\{vv_1, vv_2, \cdots, vv_m\}$ of G.
Consider the graph $G_1(U, W)$.
We have,

$$M_{\frac{1}{2}}(G_1) = \sum_{i=1}^{m} \frac{1}{\sqrt{y_i}} \quad (4.12)$$

Substitute 4.11 in 4.10,

$$R_A(G) = R_B(G) + M_{\frac{1}{2}}(G_1)[\frac{1}{\sqrt{m+2}} - \frac{1}{\sqrt{m+1}}] + \frac{1-\sqrt{2}}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{m+2}} - \frac{1}{\sqrt{2(m+1)}}$$

V. CONCLUSION

In this paper,we calculated the generalized formulae of Randic index of graphs formed on the basis of Combinations A and B. The general Randic index of G is defined as the sum of $(d_u d_v)^a$ over all edges uv of G.ie,

$$R_\alpha(G) = \sum_{uv \in E} (d_u d_v)^a$$

It may be interesting to discuss the general Randic index for above discussed various class of graphs based on Combinations different from A and B.

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