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R Index of Some Graphs

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Abstract. A topological representation of a molecule is called molecular graph. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in molecular graph theory. In this paper, the expression of the new R index of path graph, star graph, wheel graph, gear graph, helm graph are derived.

Keywords: Degree of vertex, Neighbourhood, Topological indices

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1. Introduction

A topological index is a numerical invariant that characterize the chemical properties of a molecule. The Wiener index **W(G)** is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds, which is introduced by Harold Wiener in 1947 for predicting boiling points b. p of alkanes based on the formula $b.p = \alpha W + \beta w(3) + \gamma$,where α, β, γ are empirical constants, and w(3) is called path number. It is defined as the half sum of the distances between all pairs of vertices of G. $W(G) = \frac{1}{2}\sum_{u,v\in G} d(u,v)$, where d(u,v) is the number of edges in a shortest path that connecting the vertices u & v in G[13,20]. As of now, innumerable "Molecular descriptors" are being proposed. Recently, degree based topological indices are also made a good correlation with chemical properties of a molecule. Some well-known degree based topological indices are Randic index, First and Second Zagreb indices, Reformulated first and second Zagreb indices, Atom-Bond Connectivity index, Augmented Zagreb index, Harmonic index, Geometric-arithmetic index, Sum-connectivity index, etc.[1,2,4-10,12,14-17,19,20]. The comparative testing of these well-known degrees based topological indices were given in [11]. The concept of R degree of a vertex and R index of a graph were introduced by Siileyman Ediz and computed the R degree of a vertex and R index of some well-known graphs in [18]. Throughout this paper only simple connected graphs was considered, i.e. connected graphs without self-loops and parallel edges.

2. Definitions

For a graph G, V(G) and E(G) denote the set of all vertices and edges respectively. The degree of the vertex v is defined as the number of edges incident with v and denoted by d(v). The set of all vertices which are adjacent to v is called the neighborhood of v and denoted by N(v). For a vertex v, the sum degree of v is defined as $S_v = \sum_{u \in N(v)} \deg(u)$ and for a vertex v, the multiplication degree of v is defined as $M_v = \prod_{u \in N(v)} \deg(u)$ .The R degree of a vertex v of a simple connected graph G is defined as $r(v) = S_v + M_v$. The first R index of a simple connected graph G defined as $R^1(G) = \sum_{v \in G} (r(v))^2$. The Second R index of a simple connected graph G defined as $R^2(G) = \sum_{uv \in E} r(u)\, r(v)$. The Third R index of a simple connected graph G defined as $R^3(G) = \sum_{uv \in E} [r(u) + r(v)]$

Our notation is standard and mainly taken from standard books of graph theory [3]

3. R index of some graphs

Theorem 3.1. Let P_n be the path graph with n vertices $(n \geq 3)$ then

$R^1(P_n) = 64n - 174$

$R^2(P_n) = 64n - 200$

$R^3(P_n) = 16n - 4$

Proof: Let P_n be the Path graph with n vertices and n-1 edges . ie. $|V(P_n)| = n$ and $|E(P_n)| = n - 1$ For the Pendent vertices v_1 *and* v_n , $S_{v_1} = S_{v_n} = 2 = M_{v_1} = M_{v_n} = 2$ and for the vertices v_2, v_{n-1}, $S_{v_2} = S_{v_{n-1}} = 3$ and $M_{v_2} = M_{v_{n-1}} = 2$ .For the rest of the internal vertices $S_{v_3} = ... = S_{v_{n-2}} = M_{v_3} = ... = M_{v_{n-2}} = 4$.

Hence, $r(v_2) = r(v_{n-1}) = 5$, $r(v_3) = ... = r(v_{n-2}) = 8$

After Simplification,

$R^1(P_n) = 2.4^2 + 2.5^2 + (n-4)8^2 = 64n - 174$

$R^2(P_n) = 2.5.8 + 2.4.5 + 65(n-5) = 64n - 200$

$R^3(P_n) = 2.4.5 + 2(5+8) + 16(n-5) = 16n - 4$

Theorem 3.2. Let S_n be the Star graph with n vertices $(n \geq 3)$ then

$R^1(S_n) = n^2 + 4(n-1)^3$

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

$R^3(S_n) = (n-1)(3n-2)$

Proof: Let S_n be the Star graph with n vertices and n-1 edges . ie. $|V(S_n)| = n$ and $|E(S_n)| = n-1$

For the Pendent vertices $v_1,...,v_{n-1}$, $S_{v_1} = ... = S_{v_{n-1}} = n-1 = M_{v_1} = ... = M_{v_{n-1}}$ and for the central vertex v_n, $S_{v_n} = n-1$ and $M_{v_n} = 1$.

Hence $r(v_1) = ... = r(v_{n-1}) = 2n-2$, $r(v_n) = n$

After Simplification,

$$R^1(S_n) = (n-1)(2n-2)^2 + n^2 = 4(n-1)^3 + n^2$$
$$R^2(S_n) = n(n-1)(2n-2) = 2n(n-1)^2$$
$$R^3(S_n) = (n-1)(2n-2+n) = (n-1)(3n-2)$$

Theorem 3.3. Let W_n be the Wheel graph with n vertices $(n \geq 4)$ then

$$R^1(W_n) = (n-1)(10n-4)^2 + \left(3(n-1) + 3^{n-1}\right)^2$$
$$R^2(W_n) = (n-1)(10n-4)\left(13n-7+3^{n-1}\right)$$
$$R^3(W_n) = 3(n-1)\left(11n-5+3^{n-2}\right)$$

Proof: Let W_n be the Wheel graph with n vertices and 2n-2 edges is obtained by connecting a single vertex to a vertices of a cycle of length n-1

ie. $|V(W_n)| = n$ and $|E(W_n)| = 2n-2$

For the vertices $v_1,...,v_{n-1}$, $S_{v_1} = ... = S_{v_{n-1}} = 5+n$, $M_{v_1} = ... = M_{v_{n-1}} = 9(n-1)$ and for the central vertex v_n, $S_{v_n} = 3(n-1)$ and $M_{v_n} = 3^{n-1}$.

Hence $r(v_1) = ... = r(v_{n-1}) = 5+n+9(n-1)$, $r(v_n) = 3(n-1) + 3^{n-1}$

After Simplification,

$$R^1(W_n) = (n-1)(10n-4)^2 + \left(3(n-1) + 3^{n-1}\right)^2$$
$$R^2(W_n) = (n-1)(10n-4)\left(13n-7+3^{n-1}\right)$$
$$R^3(W_n) = 3(n-1)\left(11n-5+3^{n-2}\right)$$

Theorem 3.4. Let H_n be the Helm graph with 2n-1 vertices $n \geq 4$ then

$$R^1(H_n) = (n-1)(17n-8)^2 + \left(4(n-1) + 4^{n-1}\right)^2 + 64(n-1)$$
$$R^2(H_n) = (n-1)(17n-8)\left(21n-4+4^{n-1}\right)$$
$$R^3(H_n) = 4(n-1)\left(18n-7+4^{n-2}\right)$$

Proof: Let H_n be the Helm graph with 2n-1 vertices and 3n-3 edges is obtained from the Wheel W_n by adding a pendent edge at each vertex on the rim of W_n

ie. $|V(H_n)| = 2n-1$ and $|E(H_n)| = 3n-3$

For the vertices $v_1,...,v_{n-1}$, in C_{n-1}, $S_{v_1} = ... = S_{v_{n-1}} = 8+n$,
$M_{v_1} = ... = M_{v_{n-1}} = 16(n-1)$ and for the central vertex v_n, $S_{v_n} = 4(n-1)$ and
$M_{v_n} = 4^{n-1}$. For the Pendent vertices, $S_v = 4$ and $M_v = 4$.
Hence $r(v_1) = ... = r(v_{n-1}) = 17n-8$, $r(v_n) = 4(n-1)+4^{n-1}$, $r(v_{n+1}) = ...r(v_{2n-1}) = 8$
After Simplification,

$$R^1(H_n) = (n-1)(17n-8)^2 + \left(4(n-1)+4^{n-1}\right)^2 + 64(n-1)$$
$$R^2(H_n) = (n-1)(17n-8)\left(21n-4+4^{n-1}\right)$$
$$R^3(H_n) = 4(n-1)\left(18n-7+4^{n-2}\right)$$

Theorem 3.5. Let G_n be the Helm graph with 2n+1 vertices $n \geq 4$ then

$$R^1(G_n) = (n-1)(5n-1)^2 + \left(3(n-1)+3^{n-1}\right)^2 + 225(n-1)$$
$$R^2(G_n) = 3(n-1)(5n-1)\left(3^{n-2}+n+9\right)$$
$$R^3(G_n) = 3(n-1)\left(3^{n-2}+6n+8\right)$$

Proof: Let G_n be the Gear graph with 2n+1 vertices and 3n edges is obtained by inserting an vertex between each pair of adjacent vertices on the rim of a Wheel W_n .
ie. $|V(G_n)| = 2n+1$ and $|E(G_n)| = 3n$
For the vertices $v_1,...,v_{n-1}$, in C_{n-1}, $S_{v_1} = ... = S_{v_{n-1}} = 3+n$,
$M_{v_1} = ... = M_{v_{n-1}} = 4(n-1)$ and for the central vertex v_n, $S_{v_n} = 3(n-1)$ and
$M_{v_n} = 3^{n-1}$. For the inserting vertices, $S_v = 6$ and $M_v = 9$.
Hence $r(v_1) = ... = r(v_{n-1}) = 5n-1$, $r(v_n) = 3(n-1)+3^{n-1}$, $r(v_{n+1}) = ...r(v_{2n+1}) = 15$
After Simplification,

$$R^1(G_n) = (n-1)(5n-1)^2 + \left(3(n-1)+3^{n-1}\right)^2 + 225(n-1)$$
$$R^2(G_n) = 3(n-1)(5n-1)\left(3^{n-2}+n+9\right)$$
$$R^3(G_n) = 3(n-1)\left(3^{n-2}+6n+8\right)$$

4. Conclusion

In this paper, the expression of the new R index of Path graph, Star Graph, Wheel graph, Gear graph, Helm graph are derived.

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