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On Zagreb Indices of Honeycomb Networks

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Abstract: ***The first and second Zagreb indices are defined as M_1 (G) =$\sum_{uv\in E(G)}(d_u + d_v)$ and M_2 (G) =$\sum_{uv\in E(G)}(d_u \times d_v)$ respectively, where d_u is the degree of vertex u. These are degree - based and fundamental topological indices in graph theory. In this paper degree, reverse, Revan, reduced reverse, leap, eccentricity based, first, second, third, fourth and fifth Zagreb indices of honeycomb networks and degree - based Zagreb indices of line graph of subdivision graph of honeycomb network are investigated.***

Keywords: Degree, honeycomb network, leap degree, line graph, Revan degree, reverse degree, Zagreb indices

1. Introduction

Let G be a simple, finite, connected graph with vertex set V(G) and edge set E(G). The degree of a vertex u ∈ V(G) is denoted by d_u and is the number of vertices adjacent to u. The edge connecting the vertices u and v is denoted by uv. A molecular graph is representation of the structural formula of a chemical compound in terms of graph theory whose vertices correspond to the atoms of compound and edges correspond to chemical bonds [1]. A topological index is a numeric quantity associated with a graph which characterizes the topology of graph and is invariant under graph automorphism. Zagreb indices of a graph are the mostly studied degree-based topological indices in graph theory. The parameter n of HC(n) honeycomb network is called the dimension of HC(n). The honeycomb network HC (1) is hexagon. The number of vertices and edges of HC(n) are $6n^2$ and $9n^2$–3n respectively [2]. The second Zagreb index of honeycomb network is given by ZG_2 = 3($27n^2$-21n+2) [3].Edge partition of HC(n) based on degree sum of neighbors of end vertices of each edge in 4-dimensiontional honeycomb network was presented in [4].Multiplicative topological indices of honeycomb network were computed in [5].Honeycomb networks are used in computer graphics, cellular phone base stations, image processing and as a representation of benzene of hydrocarbons in chemistry [6]. The honeycomb network can be used to study the cicumcoronene benzenoid series by analyzing the graph theoretical properties, such as the degree of vertices, the length of cycles and the symmetry of the structure [7].

Topological indices based on degrees of vertices are called degree-based topological indices. Reverse degree is defined as: c_u = Δ(G) - d_g(v)+1, where Δ(G) is maximum vertex degree among the vertices of graph G and d_g(v) is degree of vertex v. The reverse edge connecting u and v in G is denoted by uv [8]. The Revan degree of G is defined as $r_G(v) = \Delta(G) + \delta(G) - d_v$,where maximum and minimum degree of a vertex among vertices of G are denoted by Δ(G)=max{d_v|v∈V(G)}andδ(G) = min{d_v|v∈V(G)} respectively. The Revan edge connecting the Revan vertices u and v is denoted by uv [9]. Harmonic Revan vertex degree polynomial of molecular graph was proposed in [10]. The reduced reverse degree is defined as $RR_v(G) = \Delta(G) - d_v + 2$ [11].The 2-distance degree of a vertex v in G is the number of vertices which are at distance two from v and is denoted by d_2(v).The first, second and third leap Zagreb indices are defined by A.M.Naji et al.[12].Modified first leap index, leap inverse degree, leap zeroth order index and general first Zagreb index were proposed and studied by V.R.Kulli [13]. If u,v∈ V(G) then distance d(u,v) between vertices u and v is defined as the length of any shortest path in G.For a vertex u∈V(G),then its eccentricity ec(u) is defined as ec(u) = max {d(u,v)|∀u ∈V(G)}.In terms of eccentricity of a graph the first Zagreb index is defined as the sum of the squares of the eccentricities of the vertices, and second Zagreb eccentricity index is defined as the sum of the products of the eccentricities of pairs of adjacent vertices [14-17].The line graph L(G) of a graph G is a graph with vertex set which is one to one correspondence with the edge set of a graph and two vertices of L(G) are adjacent whenever the corresponding edges in G have vertex incident in common. Non-neighbor topological indices of line graph of subdivision graph of honeycomb networks were analyzed by G.R.Roshni et al.[18].

First and second Zagreb indices with edge-degree $EM_1(G) = M_1(L_G)$and $EM_2(G) = M_2(L_G)$ for circumcoronene series of benzenoid were investigated by M.R.Farahani et al.[19].Eccentricity based Zagreb indices of honeycomb network were computed in [20]. General fifth Zagreb indices of para-line graph of TUC_4C_8[6,4] lattice were computed by N.N.Swamy et al.[21]. Multiplicative degree-based topological indices of circumcoronene series were studied in [22].Molecular properties of symmetrical networks using topological polynomials were studied in [23]. A new version of Zagreb index of circumcoronene series of benzenoid was studied by M.R.Farahani [24].

The first, second, third, fourth and fifth Zagreb indices are defined as [25-26]:

$M_1(G) = \sum_{uv\in E(G)}(d_u + d_v)$. (1)

$M_2(G) = \sum_{uv\in E(G)} d_u \times d_v$. (2)

$M_3(G) = \sum_{uv\in E(G)} |d_u - d_v|$. (3)

$M_4(G) = \sum_{uv\in E(G)} d_u(d_u + d_v)$. (4)

$M_5(G) = \sum_{uv\in E(G)} d_v(d_u + d_v)$. (5)

We propose first, second, third, fourth and fifth Zagreb indices based on degree, reverse, Revan, reduced reverse, leap and eccentricity and for line graph of subdivision graph of honeycomb network. For example, the Zagreb indices based on eccentricity are defined as:

$ecM_1(G) = \sum_{uv\in E(G)}(ec_u + ec_v)$. (6)

$ecM_2(G) = \sum_{uv\in E(G)} ec_u \times ec_v$. (7)

$ecM_3(G) = \sum_{uv\in E(G)} |ec_u - ec_v|$. (8)

$ecM_4(G) = \sum_{uv\in E(G)} ec_u(ec_u + ec_v)$. (9)

$ecM_5(G) = \sum_{uv\in E(G)} ec_v(ec_u + ec_v)$, (10)

where ec_u is the eccentricity of vertex u.

All the symbols and notations used in this paper are standard and mainly taken from standard books of graph theory [27 - 29]. In this paper first, second, third, fourth and fifth Zagreb indices in degree, reverse, Revan, reduced reverse, leap and eccentricity form are proposed and degree - based Zagreb indices for line graph of subdivision graph of honeycomb network are obtained.

2. Materials and Methods

A molecular graph or a chemical graph is a graph such that its vertices correspond to the atoms and edges to the bonds. The molecular graphs of honeycomb network and line graph of subdivision graph of honeycomb networks are shown in figure 1 and 2 respectively. The first, second, third, fourth and fifth Zagreb indices are proposed in the form of degree, reverse, Revan, reduced reverse, leap and eccentricity and the corresponding Zagreb indices are computed for honeycomb network HC (3). In order to study honeycomb network topologically the vertex set V (G) and edge set E (G) are observed from figure 1. The edge partition for vertex degree and Revan degree of honeycomb network are represented in table 1 and 2 respectively. For leap degree Zagreb indices, the d_2 - distance degree with respect to each vertex are observed from figure 1. Zagreb indices for line graph of subdivision graph of honeycomb network have been computed from figure 2. Zagreb indices for honeycomb network HC (3) are graphically reprented in figure 3.

3. Results and Discussion

Degree - based Zagreb indices

By using table 1, figure 1 and formulas (1 - 5) of degree - based Zagreb indices, these indices are computed for honeycomb network.

Theorem 1. First Zagreb index of honeycomb network is $54n^2 - 30$.
Theorem 2. Second Zagreb index of honeycomb network is $81n^2 - 63n+6$.
Theorem 3. Third Zagreb index of honeycomb network is 12 (n - 1).
Theorem 4. Fourth Zagreb index of honeycomb network is $162n^2 - 150n+36$.
Theorem 5. Fifth Zagreb index of honeycomb network is $162n^2 - 90n - 24$.

Proof. This theorem is proved by using table 1 and by considering degrees of vertices. There are three edges as $E_{2,2}$, $E_{2,3}$ and $E_{3,3}$ as shown in figure 1.

$M_5(G) = \sum_{uv\in E(G)} x^{d_v(d_u+d_v)}$

$= 2(2+2)\times 6+3(2+3)12(n-1)+3(3+3)(9n^2-15n+6)$

$=162n^2 - 90n - 24$.

Reverse degree - based Zagreb indices

Theorem 1. First reverse Zagreb index of honeycomb network is $54n^2 - 30$.
Theorem 2. Second reverse Zagreb index of honeycomb network is $27n^2 - 9n+6$.
Theorem 3. Third reverse Zagreb index of honeycomb network is 12 (n - 1).
Theorem 4. Fourth reverse Zagreb index of honeycomb network is $54n^2+6n - 12$.
Theorem 5. Fifth reverse Zagreb index of honeycomb network is $54n^2 - 30n+24$.

Proof. This theorem is proved by using table 1. It is observed from figure 1 that maximum degree of a vertex among the vertices of G is $\Delta (G) = 3$. There are three edges as E_1, E_2 and E_3 as

1) $E_1= \{uv|d_u = d_v= 2\}$, $c_G (v) = \Delta (G) - d_G (v) +1$, $c_G (v) = 3 - 2+1=2$, $c_G (u) = 3 - 2+1=2$.
2) $E_2= \{uv|d_u = 2, d_v = 3\}$, $c_G (v) = \Delta (G) - d_G (v) +1$, $c_G (v) = 3 - 3+1=1$, $c_G (u) = 3 - 2+1=2$.
3) $E_3= \{uv|d_u = 3, d_v = 3\}$, $c_G (v) = \Delta (G) - d_G (v) +1$, $c_G (v) = 3 - 3+1=1$, $c_G (u) = 3 - 3+1=1$.

Fifth reverse Zagreb index can be proved as;

$rM_5(G) = \sum_{uv\in E(G)} d_v(d_u + d_v)$
$= 2(2+2)\times 6+1(2+1)12(n-1)+1(1+1)3(9n^2-11n+2)$
$=54n^2-30n+24$.

Revan degree - based Zagreb indices

Theorem 1. First Revan Zagreb index of honeycomb network is $36n^2$.
Theorem 2. Second Revan Zagreb index of honeycomb network is $36n^2+12n+6$.
Theorem 3. Third Revan Zagreb index of honeycomb network is 12 (n - 1).
Theorem 4. Fourth Revan Zagreb index of honeycomb network is $72n^2+60n - 24$.
Theorem 5. Fifth Revan Zagreb index of honeycomb network is $72n^2+36$.

Proof. There are three edges as $E_{2,2}$, $E_{2,3}$ and $E_{3,3}$ as shown in figure 1.Revan degree is defined as:
$r_u= \Delta(G) +\delta(G)-d_u$, where $\Delta(G)/\delta(G)$ is maximum/minimum vertex among the vertices of a graph and d_u is the degree of vertex u.
$RM_5(G) = \sum_{uv\in E(G)} d_v(d_u + d_v)$
$= 2(2+2)(9n^2-11n+2)+2(3+2)(12n-12)+3(3+3)6$
$= 72n^2+36$.

Reduced reverse degree - based Zagreb indices

Theorem 1. First reduced reverse Zagreb index of honeycomb network is $36n^2$.
Theorem 2. Second reduced reverse Zagreb index of honeycomb network is $36n^2+12n+6$.
Theorem 3. Third reduced reverse Zagreb index of honeycomb network is 12 (n - 1).
Theorem 4. Fourthreduced reverse Zagreb index of honeycomb network is $72n^2+60n - 24$.
Theorem 5. Fifth reduced reverse Zagreb index of honeycomb network is $72n^2+36$.

Proof. There are three edges as $E_{2,2}$, $E_{2,3}$ and $E_{3,3}$ as shown in figure 1.Reduced reverse degree is defined as: $r(r_u) = \Delta(G) - d_u+2$, where $\Delta(G)$ is maximum vertex degree among the vertices of a graph and d_u is the degree of vertex u.

$RRM_5(G) = \sum_{uv\in E(G)} d_v(d_u + d_v)$
$= 3(3+3)6+2(3+2)(12n-12)+2(2+2)(9n^2-15n+6)$
$= 72n^2+36.$

Leap degree - based Zagreb indices

Theorem 1. First leap Zagreb index of honeycomb network is 191n+108.
Theorem 2. Second leap Zagreb index of honeycomb network is 496n+266.
Theorem 3. Third leap Zagreb index of honeycomb network is 9n+6.
Theorem 4. Fourth leap Zagreb index of honeycomb network is 959n+510.
Theorem 5. Fifth leap Zagreb index of honeycomb network is 1040n+564.
Proof. The 2-distance degree of vertex u is denoted by $d_2(u)$ and these degrees of vertices are observed from figure 1.
$LM_5(G) = \sum_{uv\in E(G)} d_2(v)(d_2(u) + d_2(v))$
$= 3(3+3)6+4(3+4)(3n+2)+4(4+4)(4n+2)+6(4+6)(3n+2)+6(6+6)(9n+3)$
$= 1040n+564.$

Eccentricity - based Zagreb indices

Theorem 1. First eccentricity Zagreb index of honeycomb network HC (3) is 1350.
Theorem 2. Second eccentricity Zagreb index of honeycomb network HC (3) is 6426.
Theorem 3. Third eccentricity Zagreb index of honeycomb network HC (3) is 54.
Theorem 4. Fourth eccentricity Zagreb index of honeycomb network HC (3) is 12366.
Theorem 5. Fifth eccentricity Zagreb index of honeycomb network HC (3) is13392.
Proof. There are seven edges with eccentricity as $E_{7,7}, E_{7,8}, E_{8,9}, E_{9,9}, E_{9,10}, E_{10,11}$, and $E_{11,11}$ as shown in figure 1 for honeycomb network with n = 3. Using equation (10) we have,
$ecM_5(G) = \sum_{uv\in E(G)} ec_v(ec_u + ec_v)$
$= 7(7+7)2n+8(7+8)2n+9(8+9)4n+9(9+9)2n+10(9+10)4n+11(10+11)8n+11(11+11)2n$
$= 13392.$

Zagreb indices of line graph of subdivision graph of honeycomb network

Theorem 1. First Zagreb index of line graph of honeycomb network is $162n^2 - 114n$.
Theorem 2. Second Zagreb index of line graph of honeycomb network is $243n^2 - 201n+6$.
Theorem 3. Third Zagreb index of line graph of honeycomb network is 12n - 12.
Theorem 4. Fourth Zagreb index of line graph of honeycomb network is $58n^2 - 30n - 30$.
Theorem 5. Fifth Zagreb index of line graph of honeycomb network is $162n^2+30n - 96$.

Proof. The edge partition required to prove this theorem is obtained from figure 2. The fifth Zagreb index:
$M_5(G) = \sum_{uv\in E(G)} d_v(d_u + d_v)$
$= 2(2+2)6(n+1)+3(2+3)12(n-1)+3(3+3)(9n^2-11n+2)$
$= 162n^2+30n-96.$

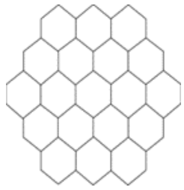

Figure 1: A honeycomb network HC (3)

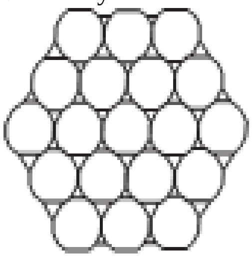

Figure 2: A Line graph of subdivision graph of honeycomb network.

Table 1: The edge partition of honeycomb network.

(d_u, d_v)	(2, 2)	(2, 3)	(3, 3)
Number of edges	6	$12(n-1)$	$9n^2 - 15n + 6$

Table 2: The Revan degree edge partition of honeycomb network.

Revan degree	(3, 3)	(3, 2)	(2, 2)
Frequency	6	12n - 12	$9n^2 - 15n + 6$

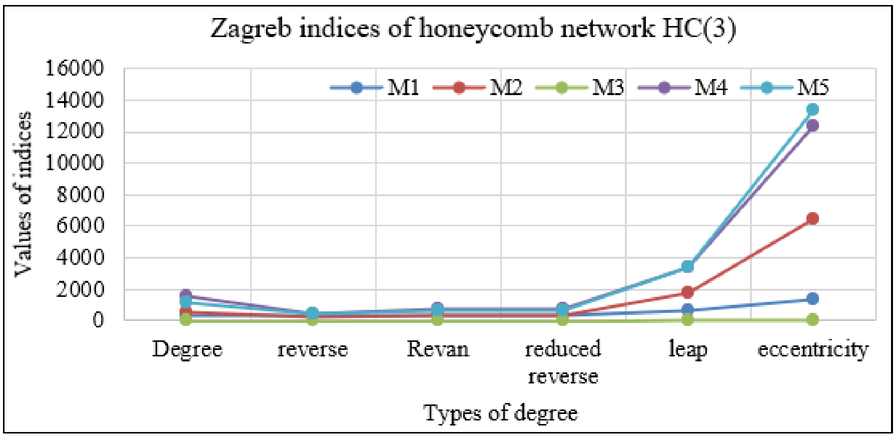

Figure 3: Graphical representation of Zagreb indices of honeycomb network

4. Conclusion

The third Zagreb index for honeycomb network HC (3) defined on degree, reverse, Revan, reduced reverse degrees and line graph of subdivision graph of honeycomb network has the same value. The degree, reverse, Revan, reduced reverse, leap and eccentricity based first, second, third, fourth and fifth Zagreb indices are graphically compared. The first, second, third, fourth and fifth Zagreb indices for line graph of subdivision graph of honeycomb network are obtained.

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