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Research paper

Vertex Hyper-Zagreb Index of Graphs

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Abstract

In this paper, we obtain the vertex hyper-Zagreb index for some composite graphs. Using the results obtained here, the vertex hyper-Zagreb index for some important classes of graphs are obtained.

Keywords: Composite graphs; F-index; Hyper-Zagreb index; Topological index ; Zagreb index; .

1. Introduction

A chemical graph is a graph whose vertices denote atoms and edges denote bonds between those atoms of any underlying chemical structure. A *topological index* for a (chemical) graph G is a numerical quantity invariant under automorphisms of G and it does not depend on the labeling or pictorial representation of the graph. Topological indices and graph invariants based on the distances between vertices of a graph or vertex degrees are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications. These indices may be used to derive quantitative structure-property or structure activity relationships (QSPR/QSAR) for more details see [Bollobs and Erds [3], Gutman and Trinajstic[13], Randic [17], Todeschini and Consonni [20]].

For a (molecular) graph G, The *first Zagreb index* $M_1(G)$ is the equal to the sum of the squares of the degrees of the vertices, and the *second Zagreb index* $M_2(G)$ is the equal to the sum of the products of the degrees of pairs of adjacent vertices, that is,

$$M_1(G) = \sum_{u\in V(G)} d_G{}^2(u) = \sum_{uv\in E(G)} (d_G(u)+d_G(v))$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

There are different types of Zagreb indices were studied by various authors. One of the important version of Zagreb indices, the vertex first and second Zagreb indices were proposed by Tavakoli et al.[10]. They are defined as

$$\overline{M}_1^*(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u)+d_G(v)),$$

$$\overline{M}_2^*(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v).$$

Shirdel et al. [9] proposed the another version of Zagreb index, namely, *hyper- Zagreb index*, which is defined as

$$HM(G) = \sum_{uv\in E(G)} (d_G(u)+d_G(v))^2.$$

Similarly, the *hyper-Zagreb co index* is defined as

$$\overline{HM}(G) = \sum_{uv\notin E(G)} (d_G(u)+d_G(v))^2.$$

In this connection, we introduce the new version of Zagreb index called vertex hyper-Zagreb index which is defined as

$$\overline{HM}_1^*(G) = \sum_{\{uv\}\subseteq E(G)} (d_G(u)+d_G(v))^2.$$

The *F -index* was introduced by Furtula and Gutman [4], and it is defined as

$$F = F(G) = \sum_{u\in V(G)} d_G{}^3(u) = \sum_{uv\in E(G)} \left(d_G{}^2(u)+d_G{}^2(u)\right)$$

They established a few basic properties of the forgotten topological index and show that it can significantly enhance the physic-chemical applicability of the first Zagreb index.

Khalifeh et al. [6] obtained the first and second Zagreb indices of the Cartesian, join, composition, disjunction and symmetric difference of two graphs. Ashrafi et al. [1] obtained the first and second Zagreb coindices of the Cartesian, join, composition, disjunction and symmetric difference of two graphs.

In Fath-Tabar [3] and shirdel et al. [9] the hyper and third Zagreb indices of some graph operations are obtained. The mathematical properties for the third and hyper-Zagreb coindices of graph operations containing the Cartesian product and composition are explained by Gao et al. [5]. Pattabiraman and Seenivasan [7] analyzed Bounds of vertex Zegreb indices of graphs for more details see[Gutman [8], Gutman [9],] Gutman ,Das [10],] Gutman , Furtula ,

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Kovijanic Vukicevic and popivoda [11], Gutman , Tomovice , [12]]. In this paper, we obtain the vertex hyper-Zagreb index for some composite graphs. Using the results obtained here, the vertex hyper-Zagreb index for some important classes of graphs are obtained.

2. Composite Graphs

Some chemically interesting graphs can be obtained by different graph operations on general or particular graphs. Thus graph operations played a important role in chemical graph theory Doslic [3]. In this view, here we obtain the vertex hyper-Zagreb indices of different types of operations of graphs.

2.1 Join

The *join* $G + H$ of graphs G and H is obtained from the disjoint union of the graphs G and H, where each vertex of G is adjacent to each vertex of H.

Theorem 1.
Let G_i be a graph with n_i vertex and m_i edges, i=1,2. Then

$$\overline{HM1}^{*}(G_1+G_2) = \overline{HM1}^{*}(G_1) + 4n_2\,\overline{M}^{*}1(G_1) + \overline{HM1}^{*}(G_2) + 4n_1\,\overline{M}^{*}1(G_2) + n_2\overline{M_1}(G_1)+n_1M_1(G_2) + n_1n_2(4n_1n_2-2n_1-2n_2+(n_1+n_2)^2) + 4(n_1+n_2)(m_1n_2+m_2n_1)+8m_1m_2.$$

Proof of theorem 1. Set $V(G_1) = \{u_1,u_2,...,u_n\}$ and $V(G_2) = \{v_1,v_2,...,v_m\}$.
By definition of the join of two graphs, one can see that,

$$d_{G1+G2}(x) = \begin{cases} dG_1(X)+n_2; & if x \in V(G_1) \\ dG_2(X)+n_1; & if x \in V(G_2) \end{cases}$$

By the definition of vertex hyper Zagreb index,

$$\begin{aligned}
\overline{HM1}^{*}(G_1+G_2) &= \sum_{\{u,v\}\subseteq V(G_1+G_2)} (d_{G_1+G_2}(u)+d_{G_1+G_2}(v))^2 \\
&= \sum_{\{u,v\}\subseteq V(G_1)} (d_{G_1+G_2}(u)+d_{G_1+G_2}(v))^2 + \sum_{\{u,v\}\subseteq V(G_2)} (d_{G_1+G_2}(u)+d_{G_1+G_2}(v))^2 + \sum_{u\in V(G_1)}\sum_{v\in v(G_2)} (d_{G_1+G_2}(u)+d_{G_1+G_2}(v))^2 \\
&= \sum_{\{u,v\}\subseteq V(G_1)} (d_{G_1}(u)+d_{G_1}(v)+2n_2)^2 + \sum_{\{u,v\}\subseteq V(G_2)} (d_{G_2}(u)+d_{G_2}(v)+2n_1)^2 + \sum_{u\in V(G_1)}\sum_{v\in v(G_2)} (d_{G_1}(u)+n_2+d_{G_2}(v)+n_1)^2 \\
&= \sum_{\{u,v\}\subseteq V(G_1)} ((d_{G_1}(u)+d_{G_1}(v))^2+4n_2^2+4n_2(d_{G_1}(u)+d_{G_1}(v)) \\
&+ \sum_{\{u,v\}\subseteq V(G_2)} ((d_{G_2}(u)+d_{G_2}(v))^2+4n_1^2+4n_1(d_{G_2}(u)+d_{G_2}(v)) \\
&+ \sum_{u\in V(G_1)}\sum_{v\in v(G_2)} (d^2{}_{G_1}(u)+d^2{}_{G_2}(v)+(n_1+n_2)^2+2d_{G_1}(u)(n_1+n_2) \\
&+ 2d_{G_2}(v)(n_1+n_2)+2d_{G_1}(u)d_{G2}(v)).
\end{aligned}$$

$$= HM^{*}{}_1(G_1) + 4n^2{}_2\,\frac{n_1(n_1-1)}{2} + 4n_2\,\overline{M}^{*}1(G_1) + HM^{*}{}_1(G_2) + 4n^2{}_1\,\frac{n_2(n_2-1)}{2} + 4n_1\,\overline{M}^{*}1(G_2) + n_2M_1(G_1) + n_1M_1(G_2) + (n_1+n_2)^2n_1n_2 + 4m_1n_2(n_1+n_2) + 4m_2(n_1+2)n_1 + 8m_1m_2.$$

Hence

$$\overline{HM1}^{*}(G_1+G_2) = \overline{HM1}^{*}(G_1) + 4n_2\,\overline{M}^{*}1(G_1) + \overline{HM1}^{*}(G_2) + 4n_1\,\overline{M}^{*}1(G_2) + n_2M_1(G_1) + n_1M_1(G_2) + n_2(4n_1n_2-2n_1-2n_2+(n_1+n_2)^2) + 4(n_1+n_2)(m_1n_2+m_2n_1) + 8m_1m_2.$$

Example 2.1. The complete bipartite graph $K_{p,q}$ can be defined as $K_{p,q} = \overline{K_p} + \overline{K_q}$. The vertex hyper-Zagreb index of $K_{p,q}$ is $pq(4pq - 2p - 2q + (p + q)^2)$.

Example 2.2. Let G be a graph with n vertices and m edges. Then

$$\overline{HM}^{*}(G+K_p) = \overline{HM1}^{*}(G) + 4p\,\overline{M}^{*}1(G) + pM_1(G) + p(p-1)^2(2p+5n-2) + np(4np-2)(n+p) + (n+p)^2) + 2(n+p)(2mp + np(p-1)) + 4mp(p-1).$$

Using Example 2.2, we obtain the following examples.

Example 2.3. The Suspension of G is defined as join of G with a single vertex. The vertex hyper-Zagreb index of $G+K_1$ is $\overline{HM1}^{*}(G) + 4\,\overline{M}^{*}1(G) + M_1(G) + n(n^2+8n-1) + 4mp(p-1)$.

Example 2.4. The fan and wheel graphs are defined as $P_n + K_1$ and $C_n + K_1$. The vertex hyper-Zagreb indices of these graphs are

(i) $\overline{HM1}^{*}(C_n+K_1) = n(n^2+24n-13)+4m(n+1)$.

(ii) $\overline{HM1}^{*}(P_n+K_1) = n(n^2+36n-71)+4m(n+1)+42$.

Example 2.5. The Cone graph $C_{n,p}$ is defined as $C_n + K_p$. So the vertex hyper Zagreb index of cone graph is given

$$\overline{HM1}^{*}(C_n+K_p) = 8n(n-1)(p+1) + 4pn + p(p-1)^2(2p+5n-2) + np(4np-2(n+p)+(n+p)^2) + 2(n+p)np(p+1))+4np(p-1).$$

2.2 Union

Let G and H be two connected graphs with V (G) and V (H) vertices, respectively. The union of G and H is the graph denoted by G ∪H with the vertex set V(G) ∪ V(H) and the edge set E(G) ∪ E(H), where V(G) and V(H) are disjoint. The degree of a vertex u in G ∪H is degree of that vertex in the components G and H that contains it. Now we obtain the vertex hyper-zagreb index of the union of two graphs.

Theorem 2. Let $\overline{HM1}^{*}(G_1 \cup G_2) = \overline{HM1}^{*}(G_1) + \overline{HM1}^{*}(G_2) + n_2M_1(G_1) + n_1M_1(G_2) + 4m_1m_2$.

Proof of theorem 2. From the structure of the G∪H, we have

$$\begin{aligned}
\overline{HM1}^{*}(G_1 \cup G_2) &= \sum_{\{u,v\}\in V(G)} (d_G(u)+d_G(v))^2 \\
&= \sum_{\{u,v\}\in V(G_1)} (d_{G1}(u)+d_{G_1}(v))^2 + \sum_{\{u,v\}\in V(G_2)} (d_{G_2}(u)+d_{G_2}(v))^2
\end{aligned}$$

$$+\sum_{u\in V(G_1)}\sum_{v\in V(G_2)}(d_{G_1}(u)+d_{G_2}(v))^2$$
$$=\overline{HM1}^{*}(G_1)+\overline{HM1}^{*}(G_2)+n_2M_1(G_1)+n_1M_1(G_2)+4m_1m_2.$$

2.3 Cartesian Product

The Cartesian product, G □ H, of the graphs G and H has the vertex set V(G □ H) =V(G) ×V(H) and (u, x)(v,y) is an edge of G □ H if u = v and xy ∈ E(H) or, uv ∈ E(G) and x = y. To each vertex u ∈ V(G), there is an isomorphic copy of H in G □ H and to each vertex v∈V(H), there is an isomorphic copy of G in G □ H.

Theorem 3. Let G_i be a graph with n_i vertex and m_i edges, i = 1, 2. Then

$$\overline{HM}(G_1\square G_2)=\frac{M_1(G_1)}{2}[2n_2^2n_1-3n_2-18m_2]+\frac{M_1(G_2)}{2}[2n_1^2n_2-3n_1-18m_1]-2n_1m_2(G_2)-2n_2m_2(G_1)-n_2F(G_1)-n_1F(G_2)+4(n_1m_2+n_2m_1)^2+8m_1m_2(n_1n_2-2)$$

The proof of the following theorem follows by applying Theorem 4.1 of [5] and Theorem 3 respectively, and using the fact that $HM(G)=\overline{HM}^{*}(G)-\overline{HM}(G)$.

Theorem 4 . Let G_i be a graph with n_i vertex and m_i edges, i = 1, 2. Then

$$\overline{HM1}^{*}(G_1\square G_2)=n_1HM(G_2)+n_2HM(G_1)+\frac{M_1(G_1)}{2}[2n_2^2n_1-3n_2+6m_2]+\frac{M_1(G_2)}{2}[2n_1^2n_2-3n_1+6m_1]-2[n_1M_2(G_2)+n_2M_2(G_1)]-[n_2F(G_1)+n_1F(G_2)]+4(n_1m_2+n_2m_1)^2+8m_1m_2(n_1n_2-2).$$

By using Theorem 4, we obtain the following examples.

Example 2.6. The C_4 -nanotorus denoted by TC_4 (m, n), is defined as the Cartesian product of two cycles.

Then $\overline{HM1}^{*}(C_n\square C_m)=4nm(8nm+1)$.

Example 2.7. The C_4 -nanotube denoted by TUC_4(m, n), is defined as the Cartesian product of two paths. Then

$$\overline{HM1}^{*}(P_n\square P_m)=4m^2[6(n^2-n)+1]-12m(n^2-n)-2(n^2-32n+5).$$

Example 2.8. The vertex hyper-Zagreb index of the Cartesian product of a path and a cycle is $\overline{HM1}^{*}(P_n\square C_m)=n^2(12m^2-9m+4)+16mn-21m+4n-4m^2(6n-1)+2$.

Example 2.9. The Ladder graph L_m made by m square is the Cartesian product of P_2 and P_m. The vertex hyper-Zagreb index of L_n is given by $\overline{HM1}^{*}(L_n)=70n^2-8n+6$.

2.4 Double Graph

Let G be a graph with V(G) = {$v_1, v_2,..., v_n$}. The vertices of the double graph G^* are given by the two sets X = { $x_1, x_2,..., x_n$} and Y = {$y_1, y_2,..., y_n$}. Thus, for each vertex v_i∈ V (G), there are two vertices x_i and y_i in V (G^*). The double graph G^* includes the initial edge set of each copy of G, and for any edge $v_i v_j$∈ E(G), two more edges $x_i y_j$ and $x_j y_i$ are added.

Theorem 5. Let G be a connected graph. Then $\overline{HM1}^{*}(G^*)=16HM(G)+16\overline{HM}(G)+16M_1(G)$.

The proof of the above theorem follows by applying Theorems 2.3 and 2.4 of [8], respectively.

2.5 Corona Product

For given graphs G and H , we define their corona product G ◦ H as the graph obtained by taking |V (G)| copies of H and joining each vertex of the i -th copy with vertex v_i∈ V (G). Obviously, |V (G ◦ H)| = |V (G)| (1 + |V (H)|) and | E(G ◦ H)| =| E(G)| + |V (G)| (|V (H)| + | E(H)|). From the structure of the corona product of two graphs, we have the degree of a vertex x in V (G_1◦ G_2) is given by

$$d_{G1\circ G2}(x)=\begin{cases}dG_1(X)+|V(G_2)|, & if x\in V(G_1)\\ dG_2(X)+1, & if x\in V(G_2,i), i=1,2,...,|V(G_1)|\end{cases}$$

where $G_{2,i}$ is the i^{th} copy of G_2

.

The following theorem is presented in [11].

Theorem 6. Let G_i be a graph with n_i vertex and m_i edges, i = 1, 2. Then

$$\overline{HM}(G_1\circ G_2)=2[\overline{M_2}(G_1)+n_2\overline{M_1}(G_1)+n_1\overline{M_1}(G_2)+\overline{M_2}(G_2)n_1]-F(G_1)-n_1F(G_2)+(n_1+n_1n_2-3n_2-1)M_1(G_1)+n_1(n_1+n_1n_2-4)M_1(G_2)+n_2^2(n_1(n_1-1)-2m_1)+n_1(n_2(n_2-1)-2m_2)+n_1n_2(8n_1m_2+3n_1n_2-8m_2-3n_2)+2(n_1-1)(4m_1m_2+2n_2m_1+2m_2^2n_1)+(n_1(n_2+1)-1)[n_1n_2^2+4n_2m_1+n_1n_2+4n_1m_2]-(6n_2^2m_1+6n_1m_2+n_1n_2(n_2^2+1)).$$

The proof of the following theorem follows by applying Theorem 2.5 of [2] and Theorem 6, respectively.

Theorem 7. Let G_i be a graph with n_i vertex and m_i edges, i=1,2.Then

$$\overline{HM1}^{*}(G_1\circ G_2)=(n_2+1)^3HM(G_1)+m_2HM(G_2)+(m_1+(n_2+1)^2\overline{HM}(G_1)+8m_1\overline{M_1}(G_2)-n_2(n_2+1)^2F(G_1)+(n_2+1)^2n_1n_2M_1(G_1)+(8m_2+n_1^2-m_1+n_2m_1(m_1-1))M_1(G_2)+16m_2^2+4m_1(2m_2-2n_2^2+5n_2)+8(n_2+1)n_1m_1(n_2+m_2)-32m_1m_2+4n_1^2(2m_2+n_2)+m_1(m_1-1)(4m_2^2+8n_2^2+16n_2m_2).$$

For a given graph G, its t -fold bristled graph Brst(G) is obtained by attaching t vertices of degree 1 to each vertex of G. This graph can be represented as the corona product of G and complement of a complete graph on t vertices. The t -fold bristled graph of a given graph is also known as its t -thorny graph.

Example 2.10. The vertex hyper-Zagreb index of the t -fold bristled graph of C_n is given by $\overline{HM1}^{*}(C_n\circ\overline{K_t})=n^2t^3+10n^2t^2-2nt^2+17n^2t-10nt-8n+8n^2$.

2.6 Composition

The composition G[H] of graphs G and H with disjoint vertex sets V (G) and V (H) and edge sets E(G) and E(H) is the graph with vertex set V(G)×V(H) and (u_1, v_1) is adjacent with (u_2,v_2) whenever (u_1 is adjacent with u_2) or (u_1= u_2 and v_1 is adjacent with v_2). From the structure of G[H], the degree of a vertex (u, v) of G[H] is given by $d_{G[H]}((u, v)) =|V (H)| d_G(u) + d_H(v)$. The following theorem is appeared in Veylaki et al [11].

Theorem 8. Let G_i be a graph with n_i vertex and m_i edges, i=1,2. Then

$$\overline{HM}(G_1[G_2])=n_2^2M_1(G_1)(n_2^2n1-2n_2-12m_2)+M_1(G_2)(n_1^2n_2-2n_1-10n_2m_1)-n_2^4M_2(G_1)$$

$-n_1M_2(G_2)- n^4{}_2F(G_1)- n_1F(G_2)$
$+ 4m_1n^2{}_2(m_1n^2{}_2+ 2m_2n_1) + 4m^2{}_2n^2{}_1$
$+ 8m_1m_2(n_1n^2{}_2-2n_2 - m_2).$

The proof of the following theorem follows by applying Theorem 2.3 of [2] and Theorem 8, respectively.

Theorem 9. Let G_i be a graph with n_i vertex and m_i edges, i=1,2. Then $\overline{\overline{HM}}{}_1^*(G_1[G_2]) = n^4{}_2HM(G_1) + n_1HM(G_2)$
$+n^2{}_2M_1(G_1)(n_2n_1-2)+M_1(G_2)n_1(n_1n_2-2)$
$-n^4{}_2M_2(G_1)-n_1M_2(G_2)-n^4{}_2F(G_1)-n_1F(G_2)$
$+4m_1n^2{}_2(m_1n^2{}_2+2m_2n_1)+4m^2{}_2n^2{}_1$
$+8m_1m_2n_2(n_1n_2-2).$

Using Theorem 9, we have the following examples.

Example 2.11. The vertex hyper-zagreb indices of $P_n[P_m]$ and $C_n[C_m]$ are given by

(i) $\overline{\overline{HM}}{}_1^*(P_n[P_m]) = 4m^4(n^2- n - 1)$
$+ m^3(20n^2+ 22n)- 4m^2(3m^2+n-7)+4n(n-1)-16m + 20mn.$

(ii) $\overline{\overline{HM}}{}_1^*(C_n[C_m]) = 4m^4(n^2-n+1)$
$+ 4m^3(5n^2- 4n) - 8m^2(n^2+ n -16)$
$- 4n^2(2m - 1) +4m(3n - 4).$

Example 2.12. The open fence graph is defined as $P_n[P_2]$. Similarly, the closed fence graph is defined as $C_n[P_2]$.
The vertex hyper-Zagreb indices of the open and closed fence graphs are given by

(i) $\overline{\overline{HM}}{}_1^*(P_n[P_2]) = 228n^2+ 132n - 168.$

(ii) $\overline{\overline{HM}}{}_1^*(C_n[P_2]) = 168n^2+ 17n.$

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