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MULTIPLICATIVE HYPER-ZAGREB INDICES AND COINDICES OF GRAPHS: COMPUTING THESE INDICES OF SOME NANOSTRUCTURES

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ABSTRACT

In this paper, we introduce the first and second multiplicative hyper-Zagreb indices of a graph. The first multiplicative hyper-Zagreb index is defined as the product of squares of the sum of the degrees of pairs of adjacent vertices. The second multiplicative hyper- Zagreb index is defined as the product of squares of the product of the degrees of pairs of adjacent vertices. Also we introduce the first and second multiplicative hyper-Zagreb coindices of a graph. In this paper, the first and second multiplicative hyper-Zagreb indices of cycles, complete graphs, complete bipartite graphs and r-regular graphs are determined. Also we compute exact formulas of the multiplicative hyper-Zagreb indices for $G = TUSC_4C_8(S)$ nanotubes, G_1 = VPHX [m, n] nanotues and G_2 = VPHY [m, n] nanotorus.

Keywords: *Molecular graph, multiplicative hyper-Zagreb index, multiplicative hyper-Zagreb coindex, nanotubes, nanotorus.*

Mathematics Subject Classification: *05C05, 05C07.*

1. INTRODUCTION

All graphs considered in this paper are finite, connected, undirected without loops and multiple edges. Any undefined term here may be found in Kulli [1].

Let $G = (V(G), E(G))$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v.

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences.

In Chemical Science, the physico-chemical properties of chemical compounds are often modeled by means of molecular graph based structure descriptors, which are referred to as topological indices.

The first and second multiplicative Zagreb indices of a graph G are defined as

$$II_1(G) = \prod_{u\in V(G)} d_G(u)^2 \text{ and } II_2(G) = \prod_{uv\in E(G)} d_G(u)d_G(v)$$

These two graph invariants are proposed by Todeshine *et al.* in [2].

In [3], Eliasi, *et al.* considered a new multiplicative version of the first Zagreb index as

$$II_1^*(G) = \prod_{uv\in E(G)} \left[d_G(u)+d_G(v)\right]$$

Recently many other multiplicative indices and coindices of graphs were studied, for example, in [4, 5, 6, 7, 8, 9, 10, 11, 12]

In this paper, we initiate a study of the multiplicative hyper-Zagreb indices of graphs.

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2. FIRST MULTIPLICATIVE HYPER-ZAGREB INDEX

We define the first multiplicative hyper-Zagreb index of a graph.

Definition 1: The first multiplicative hyper-Zagreb index of a graph G is defined as

$$HII_1(G) = \prod_{e=uv\in E(G)} \left[d_G(u) + d_G(v)\right]^2.$$

Proposition 2: Let C_n be a cycle with $n \geq 3$ vertices. Then $HII_1(C_n) = 4^{2n}$.

Proof: Let C_n be a cycle with $n \geq 3$ vertices. Consider

$$HII_1(C_n) = \prod_{uv\in E(C_n)} \left[d_{C_n}(u) + d_{C_n}(v)\right]^2 = \left[(2+2)^2\right]^n = 4^{2n}.$$

Proposition 3: Let K_n be a complete graph with n vertices. Then $HII_1(K_n) = \left[2(n-1)\right]^{n(n-1)}$.

Proof: Let K_n be a complete graph with n vertices. Then K_n has $\frac{n(n-1)}{2}$ edges. Consider

$$HII_1(K_n) = \prod_{uv\in E(K_n)} \left[d_{K_n}(u) + d_{K_n}(v)\right]^2 = \left[\{(n-1)+(n-1)\}^2\right]^{\frac{n(n-1)}{2}}$$
$$= [2(n-1)]^{n(n-1)}.$$

Proposition 4: Let $K_{m,n}$ be a complete bipartite graph with $1\leq m \leq n$. Then $HII_1(K_{m,n}) = (m+n)^{2mn}$.

Proof: Let $K_{m,n}$ be a complete bipartite graph with $1\leq m \leq n$, $m+n$ vertices and n edges. Consider

$$HII_1(K_{m,n}) = \prod_{uv\in E(K_{m,n})} \left[d_{K_{m,n}}(u) + d_{K_{m,n}}(v)\right]^2 = \left[(n+m)^2\right]^{mn}$$
$$= (m+n)^{2mn}.$$

Corollary 5: Let $K_{1,n}$ be a star. Then $HII_1(K_{1,n}) = (n+1)^{2n}$.

Theorem A [1, p.13]. Let G be an r-regular graph with n vertices. Then G has $nr/2$ edges.

Theorem 6: Let G be an r-regular graph with n vertices. Then $HII_1(G) = (2r)^{nr}$.

Proof: Let G be an r-regular graph with n vertices. By Theorem A, G has $nr/2$ edges. Consider

$$HII_1(G) = \prod_{uv\in E(G)} \left[d_G(u) + d_G(v)\right]^2 = \left[(r+r)^2\right]^{nr/2}$$
$$= (2r)^{nr}.$$

3. SECOND MULTIPLICATIVE HYPER-ZAGREB INDEX

We define the second multiplicative hyper-Zagreb index of a graph.

Definition 7: The second multiplicative hyper-Zagreb index of a graph G is defined as

$$HII_2(G) = \prod_{e=uv\in E(G)} \left[d_G(u)d_G(v)\right]^2.$$

Proposition 8: Let C_n be a cycle with $n\geq3$ vertices. Then $HII_2(C_n) = 4^{2n}$.

Proof: Let C_n be a cycle with $n\geq3$ vertices. Consider

$$HII_2(C_n) = \prod_{uv\in E(C_n)} \left[d_{C_n}(u)d_{C_n}(v)\right]^2 = \left[(2\times2)^2\right]^n = 4^{2n}.$$

Proposition 9: Let K_n be a complete graph with n vertices. Then

$$HII_2(K_n) = (n-1)^{2n(n-1)}.$$

Proof: Let K_n be a complete graph with n vertices and $\frac{n(n-1)}{2}$ edges. Consider

$$HII_2(K_n) = \prod_{uv\in E(K_n)} \left[d_{K_n}(u)d_{K_n}(v)\right]^2 = \left[\left\{(n-1)\times(n-1)\right\}^2\right]^{\frac{n(n-1)}{2}}$$
$$= (n-1)^{2n(n-1)}.$$

Proposition 10: Let $K_{m,n}$ be a complete bipartite graph with $1\leq m \leq n$. Then $HII_2(K_{m,n}) = (mn)^{2mn}$.

Proof: Let $K_{m,n}$ be a complete bipartite graph with $m+n$ vertices and mn edges. Consider

$$HII_2(K_{m,n}) = \prod_{uv\in E(K_{m,n})} \left[d_{K_{m,n}}(u)d_{K_{m,n}}(v)\right]^2 = \left[(nm)^2\right]^{mn}$$
$$= (mn)^{2mn}$$

Corollary 11: Let $K_{1,n}$ be a star. Then $KII_2(K_{1,n}) = n^{2n}$.

Theorem 12: Let G be an r-regular graph with n vertices. Then $HII_2(G) = r^{2nr}$.

Proof: Let G be a r-regular graph with n vertices. By Theorem A, G has $\frac{nr}{2}$ edges. Consider

$$HII_2(G) = \prod_{uv\in E(G)} \left[d_G(u)d_G(v)\right]^2 = \left[(r\times r)^2\right]^{nr/2}$$
$$= r^{2nr}.$$

4. FIRST AND SECOND MULTIPLICATIVE HYPER-ZAGREB COINDICES

We define the first and second multiplicative hyper-Zagreb coindices of a graph.

Definition: The first and second multiplicative hyper-Zagreb coindices of a graph G are defined as

$$\overline{HII}_1(G) = \prod_{uv\notin E(G)} \left[d_G(u)+d_G(v)\right]^2$$

$$\overline{HII}_2(G) = \prod_{uv\notin E(G)} \left[d_G(u)d_G(v)\right]^2$$

5. MULTIPLICATIVE HYPER ZAGREB INDICES OF $TUSC_4C_8(S)$ NANOTUBES

Molecular graph $TUSC_4C_8(S)$ nanotubes is a family of nanostructures that its structure consists of cycles C_4 and C_8. $TUSC_4C_8(S)$ nanotubes is denoted by $G = TUC_4C_8[m, n]$.

We compute the first and second multiplicative hyper-Zagreb indices of $G = TUC_4C_8[m, n]$ nanotubes.

Theorem 13: Let $G = TUC_4C_8[m, n]$ be the $TUSC_4C_8(S)$ nanotubes. Then

$HII_1(G) = 4^{4m}\, 5^{8m}\, 6^{24mn-4m}$

$HII_2(G) = 4^{4m}\, 5^{8m}\, 6^{24mn-4m}$.

Proof: Consider $G = TUC_4C_8[m, n]$ ($\square$ $m, n \in \mathbb{N} - \{1\}$) nanotubes. We denote the number of octagons C_8 in the first row of G by m and the number of octagons C_8 in the first column of G by n. In general case of the nanotubes, there are $8mn + 4m$ vertices/atoms and $12mn + 4m$ edges/bonds, see Figure 1.

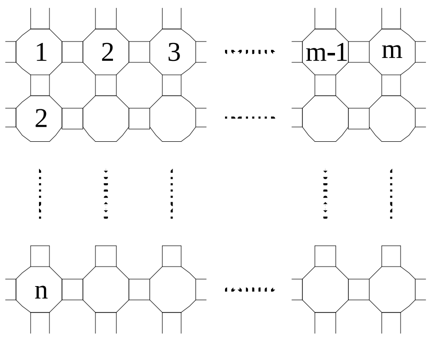

Figure-1

We have two partitions of the vertex set $V(G)$ as follows:

$V_2 = \{v \in V(G) / d_G(v) = 2\}$, $|V_2| = 2m + 2m$.

$V_3 = \{v \in V(G) / d_G(v) = 3\}$, $|V_3| = 8mn$.

By Figure 1, we have three partitions of the edge set $E(G)$ as follows:

$$E_4 = E_4^* = \{uv \in E(G) / d_G(u) = d_G(v) = 2\}, \quad |E_4| = 2m.$$

$$E_5 = E_6^* = \{uv \in E(G) / d_G(u) = 2, d_G(v) = 3\}, \quad |E_5| = |E_6^*| = 4m.$$

$$E_6 = E_9^* = \{uv \in E(G) / d_G(u) = d_G(v) = 3\}, \quad |E_6| = |E_9^*| = 12mn - 2m.$$

Now

$$\begin{aligned} HII_1(G) &= \prod_{e=uv \in E(G)} \left[d_G(u) + d_G(v)\right]^2 \\ &= \prod_{uv \in E_4} \left[d_G(u) + d_G(v)\right]^2 \times \prod_{uv \in E_5} \left[d_G(u) + d_G(v)\right]^2 \times \prod_{uv \in E_6} \left[d_G(u) + d_G(v)\right]^2 \\ &= \left(4^2\right)^{2m} \times \left(5^2\right)^{4m} \times \left(6^2\right)^{12mn-2m} \\ &= 4^{4m} \times 5^{8m} \times 6^{24mn-4m}. \end{aligned}$$

Now

$$\begin{aligned} HII_2(G) &= \prod_{e=uv \in E(G)} \left[d_G(u) d_G(v)\right]^2 \\ &= \prod_{uv \in E_4^*} \left[d_G(u) d_G(v)\right]^2 \times \prod_{uv \in E_6^*} \left[d_G(u) d_G(v)\right]^2 \times \prod_{uv \in E_9^*} \left[d_G(u) d_G(v)\right]^2 \\ &= \left(4^2\right)^{2m} \times \left(6^2\right)^{4m} \times \left(9^2\right)^{12mn-2m} \\ &= 4^{4m} \times 6^{8m} \times 9^{24mn-4m}. \end{aligned}$$

6. MULTIPLICATIVE HYPER-ZAGREB INDICES OF *V*-PHENLENIC NANOTUES AND NANOTORUS

Chemical Structures *V*-Phenylenic nanotubes and *V*-Phenylenic nanotorus are widely used in Medical Science and Pharmaceutical field. Thus we study multiplicative hyper-Zagreb indices of these molecular structures from a mathematical point of view. In this section, we consider the structures of *V*-Phenylenic nanotubes $VPHX[m, n]$ and *V*-Phenylenic nanotorus $VPHY[m, n]$ (□ $m, n \in \mathbb{N} - \{1\}$) and compute their multiplicative hyper-Zagreb indices.

Molecular graphs *V*-Phenylenic nanotubes and *V*-Phenylenic nanotorus are two families of nanostructures that their structures consist of cycles C_4, C_6 and C_8 by different compounds.

We determine the first and second multiplicative hyper-Zagreb indices of $G_1 = VPHX[m, n]$ nanotubes.

Theorem 14: Let $G_1 = VPHX[m, n]$ (□ $m, n \in \mathbb{N} - \{1\}$) be the *V*-Phenylenic nanotubes. Then

$HII_1(G_1) = 5^{8m} \times 6^{18mn - 10m}$

$HII_2(G_1) = 6^{8m} \times 9^{18mn - 10m}$.

Proof: Consider $G_1 = VPHX[m, n]$ (□ $m, n \in \mathbb{N} - \{1\}$) nanotubes. We denote the number of hexagons in the first row of G_1 by m and the number of hexagons in the first column of G_1 by n. In general case of this nanotubes, there are $6mn$ vertices/atoms and $9mn - m$ edges/bonds, see Figure 2.

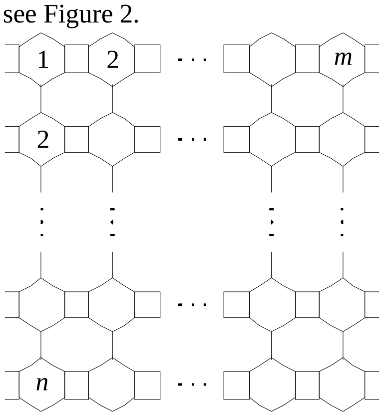

Figure-2

From the structure of G_1, we have two partitions of the vertex set $V(G_1)$ as follows:

$$V_2 = \{v \in V(G_1) : d_{G_1}(v) = 2\}, \qquad |V_2| = 2m.$$
$$V_3 = \{v \in V(G_1) : d_{G_1}(v) = 3\}, \qquad |V_3| = 6mn - 2m.$$

Also from the structure of G_1, we have two partitions of the edge set $E(G_1)$ as follows:

$$E_5 = E_6^* = \{e = uv \in E(G_1) : d_G(u) = 2, d_G(v) = 2\}, \quad |E_5| = |E_6^*| = 4m.$$
$$E_6 = E_9^* = \{e = uv \in E(G_1) : d_{G_1}(u) = d_{G_1}(v) = 3\}, \quad |E_6| = |E_9^*| = 9mn - 5m.$$

Now

$$\begin{aligned} HII_1(G_1) &= \prod_{e=uv \in E(G_1)} \left[d_{G_1}(u) + d_{G_1}(v)\right]^2 \\ &= \prod_{uv \in E_5} \left[d_{G_1}(u) + d_{G_1}(v)\right]^2 \times \prod_{uv \in E_6} \left[d_{G_1}(u) + d_{G_1}(v)\right]^2 \\ &= \left(5^2\right)^{4m} \times \left(6^2\right)^{9mn-2m} \\ &= 5^{8m} \times 6^{18mn-10m}. \end{aligned}$$

$$\begin{aligned} HII_2(G_1) &= \prod_{e=uv \in E(G_1)} \left[d_{G_1}(u) d_{G_1}(v)\right]^2 \\ &= \prod_{uv \in E_6^*} \left[d_{G_1}(u) d_{G_1}(v)\right]^2 \times \prod_{uv \in E_9^*} \left[d_{G_1}(u) d_{G_1}(v)\right]^2 \\ &= \left(6^2\right)^{4m} \times \left(9^2\right)^{9mn-5m} \\ &= 6^{8m} \times 9^{18mn-10m}. \end{aligned}$$

Now we compute the first and second multiplicative hyper-Zagreb indices of $G_2 = VPHY[m, n]$ nanotorus.

Theorem 15: Let $G_2 = VPHY[m, n]$ ($\forall\, m, n \in \mathbb{N} - \{1\}$) be the V-Phenylenic nanotorus. Then

$HII_1(G_2) = 6^{18mn}$.
$HII_2(G_2) = 9^{18mn}$.

Proof: Consider $G_2 = VPHY[m, n]$ ($\forall\, m, n \in \mathbb{N} - \{1\}$) nanotorus. We denote the number of hexagons in the first row of G_2 by m and the number of hexagons in the first column of G_2 by n. In general case of this nanotorus, there are $6mn$ vertices/atoms and $9mn$ edges/bonds, see Figure 3.

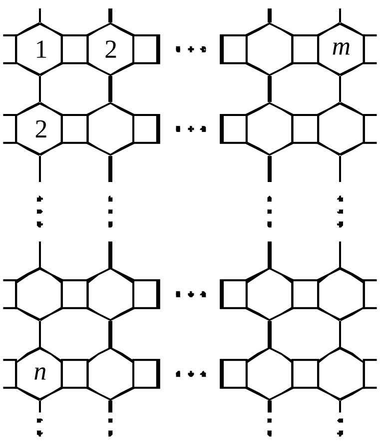

Figure-3

From the structure G_2, there is only one partition of the vertex set $V(G_2)$ as follows:

$$V_3 = \{v \in V(G_2) : d_{G_2}(v) = 3\}, \quad |V_3| = 6mn.$$

Also from the structure of G_2, there is only one partition of the edge set $E(G_2)$ as follows:

$$E_6 = E_9^* = \{uv \in E(G_2) : d_{G_2}(u) = d_{G_2}(v) = 3\}, \quad |E_6| = |E_9^*| = 9mn.$$

Now $$HII_1(G_2) = \prod_{e=uv\in E(G_2)} \left[d_{G_2}(u) + d_{G_2}(v)\right]^2$$
$$= \prod_{uv\in E_6} \left[d_{G_2}(u) + d_{G_2}(v)\right]^2$$
$$= \left(6^2\right)^{9mn} = 6^{18mn}.$$

$$HII_2(G_2) = \prod_{e=uv\in E(G_2)} \left[d_{G_2}(u) d_{G_2}(v)\right]^2$$
$$= \prod_{uv\in E_9^*} \left[d_{G_2}(u) d_{G_2}(v)\right]^2$$
$$= \left(9^2\right)^{9mn} = 9^{18mn}.$$

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