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ON THE HYPER-ZAGREB COINDEX OF SOME GRAPHS

MOHAMMED SAAD ALSHARAFI[1,*], MAHIOUB MOHAMMED SHUBATAH[2] , ABDU QAID ALAMERI[3]

[1]Department of Mathematics, Faculty of Education, Art and Science, University of Sheba Region, Yemen

[2]Department of Studies in Mathematics, Faculty of Science and Education, University of AL-Baida, Yemen

[3]Department of BME, Faculty of Engineering, University of Science and Technology, Yemen

Abstract. A topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph. In this paper some basic mathematical operation for the hyper Zagreb coindices of graph containing the tensor product $G_1 \otimes G_2$, join $G_1 + G_2$, strong product $G_1 * G_2$, disjunction $G_1 \vee G_2$ and symmetric difference $G_1 \oplus G_2$ will be explained. Moreover we studied the expression for the hyper-Zagreb coindex of titania $TiO_2[n,m]$ nanotubes and molecular graph of nanotorus have been derived. These explicit formulae can correlate the chemical structure of titania nanotubes and molecular graph of nanotorus to information about their physical structure.

Keywords: Zagreb index; Zagreb coindex; Hyper-Zagreb index; Hyper-Zagreb coindex; forgotten index; graph operation.

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1. Introduction

A topological index is a numerical value for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. It is well known that many

*Corresponding author
E-mail address: alsharafi205010@gmail.com
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graphs of general and in particular of chemical, interests arise from simpler graphs via various graph operations. Topological indices in isomer discrimination, structure-property relationship, structure-activity relationship and pharmaceutical drug design have been found to be very useful in chemistry , biochemistry and nanotechnology[9]. Throughout this paper, we consider a finite connected graph G that has no loops or multiple edges with vertex and edge sets $V(G)$, and $E(G)$, respectively. For a graph G, the degree of a vertex u is the number of edges incident to u, denoted by $\delta_G(u)$. The complement of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent, i.e., connected by an edge uv, if and only if they are not adjacent in G. Hence, $uv \in E(\overline{G})$, if and only if $uv \notin E(G)$. Obviously $E(G) \cup E(\overline{G}) = E(K_n)$, and $\overline{m} = |E(\overline{G})| = \binom{n}{2} - m$, the degree of a vertex u in $\overline{G}$, is the number of edges incident to u, denoted by $\delta_{\overline{G}}(u) = n-1-\delta_G(u)$, [16]. The first and second Zagreb indices have been introduced by Gutman and Trinajestic in 1972 [15]. They are respectively defined as:

$$M_1(G) = \sum_{v\in V(G)} {\delta_G}^2(v) = \sum_{uv\in E(G)} [\delta_G(u) + \delta_G(v)], \qquad M_2(G) = \sum_{uv\in E(G)} \delta_G(u)\,\delta_G(v),$$

The first and second Zagreb coindices have been introduced by A.R. Ashrafi, T. Doslic, and A. Hamzeh in 2010 [5]. They are respectively defined as:

$$\overline{M}_1(G) = \sum_{uv\notin E(G)} [\delta_G(u) + \delta_G(v)], \qquad \overline{M}_2(G) = \sum_{uv\notin E(G)} \delta_G(u)\,\delta_G(v),$$

In 2013, G.H. Shirdel, H. Rezapour and A.M. Sayadi [10] iintroduced distance-based of Zagreb indices named Hyper-Zagreb index which is defined as:

$$HM(G) = \sum_{uv\in E(G)} [\delta_G(u) + \delta_G(v)]^2$$

In 2016, Maryam Veylaki, et al [16] introduced distance-based of Zagreb indices named Hyper-Zagreb coindex which is defined as :

$$\overline{HM}(G) = \sum_{uv\notin E(G)} [\delta_G(u) + \delta_G(v)]^2$$

Furtula and Gutman in 2015 introduced forgotten index (F-index) [8] which defined as:

$$F(G) = \sum_{uv\in E(G)} \left({\delta_G}^2(u) + {\delta_G}^2(v)\right)$$

N. De, S.M.A. Nayeem and A. Pal. in 2016 defined forgotten coindex (F-coindex)[9]. which defined as:

$$\overline{F}(G) = \sum_{uv \notin E(G)} \left({\delta_G}^2(u) + {\delta_G}^2(v) \right)$$

Then, Veylaki et al.[16] and Basavanagoud et al. [7] computed the hyper Zagreb coindices of the Cartesian product and composition of two graphs. Here we continue this line of research by exploring the behavior of the hyper Zagreb coindices under several important operations such as disjunction, symmetric difference, join, tensor product and strong product. The results are applied to molecular graph of nanotorus and titania nanotubes. In recent years, there has been considerable interest in general problems of determining topological indices and them operations [1, 2, 3, 19, 20].

2. Preliminaries

In this section we give some basic and preliminary concepts which we shall use later.

Lemma 2.1:[4] Let G_1 and G_2 be two connected graphs with $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, $|E(G_1)| = m_1$, and $|E(G_2)| = m_2$. Then

1. $|V(G_1 \times G_2)| = |V(G_1 \vee G_2)| = |V(G_1 \circ G_2)| = |V(G_1 \otimes G_2)| = |V(G_1 * G_2)| =$ $|V(G_1 \oplus G_2)| = n_1 n_2,\ |V(G_1 + G_2)| = n_1 + n_2,$

2. $|E(G_1 \times G_2)| = m_1 n_2 + n_1 m_2, \quad |E(G_1 * G_2)| = m_1 n_2 + n_1 m_2 + 2m_1 m_2$,

   $|E(G_1 + G_2)| = m_1 + m_2 + n_1 n_2, \quad |E(G_1 \circ G_2)| = m_1 {n_2}^2 + m_2 n_1,$

   $|E(G_1 \vee G_2)| = m_1 {n_2}^2 + m_2 {n_1}^2 - 2m_1 m_2, \qquad |E(G_1 \otimes G_2)| = 2m_1 m_2,$

   $|E(G_1 \oplus G_2)| = m_1 {n_2}^2 + m_2 {n_1}^2 - 4m_1 m_2.$

3. $\delta_{G_1 * G_2}(u,v) = \delta_{G_1}(u) + \delta_{G_2}(v) + \delta_{G_1}(u)\delta_{G_2}(v).$

Corollary 2.2:[15] The first Zagreb index of some well-known graphs: For path graph P_n and cycle graph C_n, with $n : n \geq 3$ vertices :

$$M_1(C_n) = 4n, \quad M_1(P_n) = 4n - 6.$$

Corollary 2.3:[10, 6] The Hyper-Zagreb index of some well-known graphs: For path P_n and cycle graphs C_n, with $n,m \geq 3$ vertices :

$$HM(C_n) = 16n, \quad HM(P_n) = 16n-30, \quad M(P_n \times C_m) = 128nm - 150m, \quad HM(C_n \times C_m) = 128nm.$$

Corollary 2.4:[16] The Hyper-Zagreb coindex of path P_n and cycle graphs C_n, with $n : n \geq 3$ vertices are:

$$\overline{HM}(C_n) = 8n(n-3), \quad \overline{HM}(P_n) = 8n^2 - 38n + 46.$$

Corollary 2.5:[7] The Hyper-Zagreb coindex of some well-known graphs:

For a path graph and a cycle graph with $m,n \geq 3$, vertices :

(1) $\overline{HM}(P_n \times P_m) =$
$4(2nm-n-m)^2 + (nm-1)(16nm-14n-14m+8) - 144nm + 164n + 164m - 152,$

(2) $\overline{HM}(P_n \times C_m) = 4(2nm-m)^2 + (nm-1)(16nm-14m) - 144nm + 164m,$

(3) $\overline{HM}(C_n \times C_m) = 32nm(nm-5.$

Proposition 2.6:[5] Let G be a simple graph on n vertices and m edges. Then.

$$M_1(\overline{G}) = M_1(G) + 2(n-1)(\overline{m}-m), \quad \overline{M}_1(G) = 2m(n-1) - M_1(G), \quad \overline{M}_1(\overline{G}) = 2(n-1)\overline{m} - M_1(\overline{G}).$$

Theorem 2.7:[11] Let G be a simple graph on n vertices and m edges. Then.

$$\begin{aligned}
HM(\overline{G}) &= 4(n-1)^2\overline{m} - 4(n-1)\overline{M}_1(G) + \overline{HM}(G), \\
\overline{HM}(G) &= (n-2)M_1(G) + 4m^2 - HM(G), \\
&= HM(\overline{G}) - 4(n-1)M_1(\overline{G}) + 4\overline{m}(n-1)^2, \\
&= 2\overline{M}_2(G) + (n-1)M_1(G) - F(G), \\
\overline{HM}(\overline{G}) &= 4m(n-1)^2 - 4(n-1)M_1(G) + HM(G), \\
&= 4\overline{m}^2 + (n-2)M_1(\overline{G}) - HM(\overline{G}).
\end{aligned}$$

Proposition 2.8:[16] Let G_1, G_2 be two simple graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\overline{HM}(G_1+G_2)=\overline{HM}(G_1)+\overline{HM}(G_2)+4(n_1\overline{M}_1(G_2)+n_2\overline{M}_1(G_1))+4[n_1^2\overline{m}_2+n_2^2\overline{m}_1].$$

Proposition 2.9:[7] Let G_1, G_2 be two simple graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}\overline{HM}(G_1\times G_2) &= 2[2(n_1m_2+n_2m_1)^2-4m_1m_2-n_1M_2(G_2)-n_2M_2(G_1)\\ &- [(3m_2+(1/2)n_2)M_1(G_1)+(3m_1+(1/2)n_1)M_1(G_2)]]+(n_1n_2-1)[n_1M_1(G_2)\\ &+ n_2M_1(G_1)+8m_1m_2]-[n_2F(G_1)+n_1F(G_2)+6m_2M_1(G_1)+6m_1M_1(G_2)],\end{aligned}$$

$$\begin{aligned}\overline{HM}(G_1\circ G_2) &= 2[2m_1n_2^2(m_1n_2^2+2m_2n_1)+2m_2^2n_1^2-4m_1m_2(n_2+m_2)\\ &- n_2^2(3m_2+n_2/2)M_1(G_1)-(n_1/2+2n_2m_1)M_1(G_2)-(n_2^4M_2(G_1)+n_1M_2(G_2))]\\ &+ (n_1n_2-1)[n_2^3M_1(G_1)+n_1M_1(G_2)+8n_2m_1m_2]-[n_2^4F(G_1)+n_1F(G_2)\\ &+ 6n_2^2m_2M_1(G_1)+6n_2m_1M_1(G_2)].\end{aligned}$$

3. Main Results

In this section, we study the Hyper-Zagreb coindex of various graph binary operations such as Cartesian product $G_1\times G_2$, composition $G_1\circ G_2$, disjunction $G_1\vee G_2$, symmetric difference $G_1\oplus G_2$, join G_1+G_2, tensor product $G_1\otimes G_2$, and strong product $G_1 * G_2$, of graphs. We use the notation $V(G_i)$ for the vertex set, $E(G_i)$ for the edge set, n_i for the number of vertices and m_i for the number of edges of the graph G_i respectively. All graphs here offer are simple graphs.

Tensor product

The tensor product $G_1\otimes G_2$, of two simple and connected graphs G_1 and G_2 is the graph with vertex set $V(G_1)\times V(G_2)$ and $E(G_1\oplus G_2)=(u_1,u_2)(v_1,v_2)|u_1v_1\in E(G_1)$ and $u_2v_2\in E(G_2)$.

Theorem 3.1: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\overline{HM}(G_1\otimes G_2)=16m_1^2m_2^2+(n_1n_2-2)M_1(G_1)M_1(G_2)-F(G_1)F(G_2)-2M_2(G_1)M_2(G_2).$$

Proof. By using Theorem 2.7. we have $\overline{HM}(G_1 \otimes G_2) = (|V(G_1 \otimes G_2)| - 2)M_1(G_1 \otimes G_2) + 4|E(G_1 \otimes G_2)|^2 - HM(G_1 \otimes G_2)$, and since $M_1(G_1 \otimes G_2) = M_1(G_1)M_1(G_2)$, given in [12]. $HM(G_1 \otimes G_2) = F(G_1)F(G_2) + 2M_2(G_1)M_2(G_2)$, given in [13].
$|E(G_1 \otimes G_2)| = 2m_1m_2, \quad |V(G_1 \otimes G_2)| = n_1n_2$ given in Lemma 2.1. which is complete the proof.

Proposition 3.2: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned} \overline{HM}(\overline{G_1 \otimes G_2}) &= 8m_1m_2(n_1n_2-1)^2 - 4(n_1n_2-1)M_1(G_1)M_1(G_2) + F(G_1)F(G_2) \\ &+ 2M_2(G_1)M_2(G_2). \end{aligned}$$

Join

The join $G_1 + G_2$, of two simple and connected graphs G_1 and G_2 is a graph with vertex set $V(G_1+G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_1) \cup \{uv | u \in V(G_1), v \in V(G_2)\}$.

Theorem 3.3: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned} \overline{HM}(G_1+G_2) &= 4[m_1+m_2+n_1n_2]^2 + (n_1+n_2-2)[M_1(G_1)+M_1(G_2)+n_1n_2^2+n_2n_1^2 \\ &+ 4m_1n_2+4m_2n_1] - [HM(G_1)+HM(G_2)+5(n_1M_1(G_2)+n_2M_1(G_1)) \\ &+ 8[n_1^2m_2+n_2^2m_1+m_1m_2] + n_1n_2[(n_2+n_1)^2+4(m_1+m_2)]]. \end{aligned}$$

Proof. By using Theorem 2.7. we have

$$\overline{HM}(G_1+G_2) = (|V(G_1+G_2)|-2)M_1(G_1+G_2) + 4|E(G_1+G_2)|^2 - HM(G_1+G_2),$$

and since $M_1(G_1+G_2) = M_1(G_1)+M_1(G_2)+n_1n_2^2+n_2n_1^2+4m_1n_2+4m_2n_1$, given in [12]. $HM(G_1+G_2) = HM(G_1)+HM(G_2)+5(n_1M_1(G_2)+n_2M_1(G_1))+8[n_1^2m_2+n_2^2m_1+m_1m_2]+n_1n_2[(n_2+n_1)^2+4(m_1+m_2)]$, given in [10]. $|E(G_1+G_2)| = m_1+m_2+n_1n_2, \quad |V(G_1+G_2)| = n_1+n_2$ given in Lemma 2.1. which is complete the proof.

Proposition 3.4: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}\overline{HM}(\overline{G_1+G_2}) &= 4(m_1+m_2+n_1n_2)(n_1+n_2-1)^2-4(n_1+n_2-1)[M_1(G_1)+M_1(G_2)+n_1n_2^2 \\ &+ n_2n_1^2+4m_1n_2+4m_2n_1]+HM(G_1)+HM(G_2)+5(n_1M_1(G_2)+n_2M_1(G_1)) \\ &+ 8[n_1^2m_2+n_2^2m_1+m_1m_2]+n_1n_2[(n_2+n_1)^2+4(m_1+m_2)].\end{aligned}$$

Strong product

The strong product $G_1 * G_2$, of two simple and connected graphs G_1 and G_2 is a graph with vertex set $V(G_1 * G_2) = V(G_1) \times V(G_2)$ and any two vertices $((u_1, v_1)$ and $((u_2, v_2)$ are adjacent if and only if $\{\ u_1 = u_2 \in V(G_1)$ and $v_1v_2 \in E(G_2)\ \}$ or $\{\ v_1 = v_2 \in V(G_2)$ and $u_1u_2 \in E(G_1)\ \}$.

Proposition 3.5: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$M_1(G_1 * G_2) = (n_2+6m_2)M_1(G_1)+8m_2m_1+(6m_1+n_1)M_1(G_2)+2M_1(G_1)M_1(G_2)$$

Proof. By Definitions of the Zagreb index,strong product $G_1 * G_2$ and by Lemma 2.1.

$$\begin{aligned}& M_1(G_1 * G_2) \\ = & \sum_{(a,c)(b,d)\in E(G_1*G_2)} [\delta_{G_1*G_2}(a,c)+\delta_{G_1*G_2}(b,d)] \\ = & \sum_{ab\in E(G_1)} \sum_{c=d\in V(G_2)} [\delta_{G_1}(a)+\delta_{G_1}(b)+\delta_{G_1}(a)\delta_{G_2}(c)+\delta_{G_1}(b)\delta_{G_2}(d)+\delta_{G_2}(c)+\delta_{G_2}(d)] \\ + & \sum_{a=b\in V(G_1)} \sum_{cd\in E(G_2)} [\delta_{G_1}(a)+\delta_{G_1}(b)+\delta_{G_1}(a)\delta_{G_2}(c)+\delta_{G_1}(b)\delta_{G_2}(d)+\delta_{G_2}(c)+\delta_{G_2}(d)] \\ + & \sum_{ab\in E(G_1)} \sum_{cd\in E(G_2)} [\delta_{G_1}(a)+\delta_{G_1}(b)+\delta_{G_1}(a)\delta_{G_2}(c)+\delta_{G_1}(b)\delta_{G_2}(d)+\delta_{G_2}(c)+\delta_{G_2}(d)] \\ = & (n_2+6m_2)M_1(G_1)+8m_2m_1+(6m_1+n_1)M_1(G_2)+2M_1(G_1)M_1(G_2).\end{aligned}$$

Theorem 3.6: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}
& \overline{HM}(G_1 * G_2) \\
= \; & 4(m_1n_2 + n_1m_2 + 2m_1m_2)^2 + (n_1n_2 - 2)[(n_2 + 6m_2)M_1(G_1) + 8m_2m_1 \\
+ \; & (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)] - [HM(G_1) + n_1HM(G_2) + 5n_2M_1(G_1) \\
+ \; & 5n_1M_1(G_2) + 4n_2m_1[2n_2 + 1] + 8m_2[n_1 + m_1] + n_1n_2(n_2^3 + 2n_2 + 4m_2)].
\end{aligned}$$

Proof. By using Theorem 2.7. we have $\overline{HM}(G_1 * G_2) = (|V(G_1 * G_2)| - 2)M_1(G_1 * G_2) + 4|E(G_1 * G_2)|^2 - HM(G_1 * G_2)$, and since $M_1(G_1 * G_2) = (n_2 + 6m_2)M_1(G_1) + 8m_2m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)$, given in Proposition 3.7. $HM(G_1 * G_2) = HM(G_1) + n_1HM(G_2) + 5n_2M_1(G_1) + 5n_1M_1(G_2) + 4n_2m_1[2n_2 + 1] + 8m_2[n_1 + m_1] + n_1n_2[n_2^3 + 2n_2 + 4m_2]$, given in [10]. $|E(G_1 * G_2)| = m_1n_2 + n_1m_2 + 2m_1m_2$, $|V(G_1 * G_2)| = n_1n_2$ given in Lemma 2.1. which is complete the proof.

Proposition 3.7: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}
\overline{HM}(\overline{G_1 * G_2}) = \; & 4(m_1n_2 + n_1m_2 + 2m_1m_2)(n_1n_2 - 1)^2 - 4(n_1n_2 - 1)[(n_2 + 6m_2)M_1(G_1) \\
+ \; & 8m_2m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)] + HM(G_1) \\
+ \; & n_1HM(G_2) + 5n_2M_1(G_1) + 5n_1M_1(G_2) + 4n_2m_1[2n_2 + 1] + 8m_2[n_1 + m_1] \\
+ \; & n_1n_2[n_2^3 + 2n_2 + 4m_2].
\end{aligned}$$

Cartesian product

The Cartesian product $G_1 \times G_2$, of two simple and connected graphs G_1 and G_2 has the vertex set$V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and $(a,x)(b,y)$ is an edge of $G_1 \times G_2$ if $a = b$ and $xy \in E(G_2)$, or $ab \in E(G_1)$ and $x = y$.

Proposition 3.8: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}
\overline{HM}(\overline{G_1 \times G_2}) = \; & 4(m_1n_2 + m_2n_1)(n_1n_2 - 1)^2 - 4(n_1n_2 - 1)(n_2M_1(G_1) + n_1M_1(G_2) \\
+ \; & 8m_1m_2) + n_2HM(G_1) + n_1HM(G_2) + 12m_1M_1(G_2) + 12m_2M_1(G_1).
\end{aligned}$$

Composition

The composition $G_1 \circ G_2$, of two simple and connected graphs G_1 and G_2 with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$ is the graph with vertex set $V(G_1) \times V(G_2)$ and $u = (u_1, v_1)$ is adjacent with $v = (u_2, v_2)$ whenever (u_1 is adjacent with u_2) or $\{u_1 = u_2$ and v_1 is adjacent with $v_2\}$.

Proposition 3.9: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}\overline{HM}(\overline{G_1 \circ G_2}) &= 4[m_1 n_2^2 + m_2 n_1](n_1 n_2 - 1)^2 - 4(n_1 n_2 - 1)[n_2^3 M_1(G_1) + n_1 M_1(G_2) + 8n_2 m_2 m_1] \\ &+ n_2^4 HM(G_1) + n_1 HM(G_2) + 12 n_2^2 m_2 M_1(G_1) + 10 n_2 m_1 M_1(G_2) + 8 m_2 m_1.\end{aligned}$$

Disjunction

The disjunction $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and (u_1, v_1) is adjacent with (u_2, v_2), whenever $(u_1, u_2) \in E(G_1)$ or $(v_1, v_2) \in E(G_2)$.

Theorem 3.10: Let G_1, G_2 be two simple graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}\overline{HM}(G_1 \vee G_2) &= 4[m_1 n_2^2 + m_2 n_1^2 - 2m_1 m_2]^2 + (n_1 n_2 - 2)[(n_1 n_2^2 - 4m_2 n_2) M_1(G_1) \\ &+ M_1(G_2) M_1(G_1) + (n_2 n_1^2 - 4m_1 n_1) M_1(G_2) + 8 m_1 m_2 n_1 n_2] \\ &- [[n_1^4 - 2n_2^2 m_2] HM(G_2) + [n_2^4 - 2n_2^2 m_2] HM(G_1) + 5 n_1 M_1(G_1) F(G_2) \\ &+ 5 n_2 M_1(G_2) F(G_1) + 10 n_2^2 m_2 n_1 M_1(G_1) + 10 n_2 n_1^2 m_1 M_1(G_2) \\ &+ 8 n_2^2 m_2 m_1 + 8 n_1^2 m_1 m_2 - 8 n_2 m_1^2 M_1(G_2) - 8 n_1 m_2^2 M_1(G_1) \\ &- 4 n_1^2 m_1 F(G_2) - 4 n_2^2 m_2 F(G_1) - 8 n_1^2 m_1 M_2(G_2) - 8 n_2^2 m_2 M_2(G_1) \\ &+ 8 m_1 M_2(G_2) + 8 m_2 M_2(G_1) - 8 n_2 n_1 M_1(G_1) M_1(G_2) + 4 n_2 M_2(G_1) M_1(G_2) \\ &+ 4 n_1 M_2(G_2) M_1(G_1) - 2F(G_1) F(G_2) - 4 M_2(G_1) M_2(G_2)].\end{aligned}$$

Proof. By Theorem 2.7. we have $\overline{HM}(G_1 \vee G_2) = (|V(G_1 \vee G_2)| - 2) M_1(G_1 \vee G_2) + 4|E(G_1 \vee G_2)|^2 - HM(G_1 \vee G_2)$, and since $M_1(G_1 \vee G_2) = (n_1 n_2^2 - 4m_2 n_2) M_1(G_1) + M_1(G_2) M_1(G_1) +$

$(n_2n_1^2-4m_1n_1)M_1(G_2)+8m_1m_2n_1n_2$, given in [15]. And by [13] we have:

$$\begin{aligned}
HM(G_1\vee G_2) &= [n_1^4-2n_2^2m_2]HM(G_2)+[n_2^4-2n_2^2m_2]HM(G_1)+5n_1M_1(G_1)F(G_2)\\
&+ 5n_2M_1(G_2)F(G_1)+10n_2^2m_2n_1M_1(G_1)+10n_2n_1^2m_1M_1(G_2)\\
&+ 8n_2^2m_2m_1+8n_1^2m_1m_2-8n_2m_1^2M_1(G_2)-8n_1m_2^2M_1(G_1)\\
&- 4n_1^2m_1F(G_2)-4n_2^2m_2F(G_1)-8n_1^2m_1M_2(G_2)-8n_2^2m_2M_2(G_1)\\
&+ 8m_1M_2(G_2)+8m_2M_2(G_1)-8n_2n_1M_1(G_1)M_1(G_2)+4n_2M_2(G_1)M_1(G_2)\\
&+ 4n_1M_2(G_2)M_1(G_1)-2F(G_1)F(G_2)-4M_2(G_1)M_2(G_2).
\end{aligned}$$

$|E(G_1\vee G_2)|=m_1{n_2}^2+m_2{n_1}^2-2m_1m_2, \quad |V(G_1\vee G_2)|=n_1n_2$ given in Lemma 2.1. which is complete the proof.

Proposition 3.11: Let G_1,G_2 be two simple connected graphs with n_1,n_2 vertices and m_1,m_2 edges, respectively, Then.

$$\begin{aligned}
\overline{HM}(\overline{G_1\vee G_2}) &= 4[m_1n_2^2+m_2n_1^2-2m_1m_2](n_1n_2-1)^2\\
&- 4(n_1n_2-1)[(n_1n_2^2-4m_2n_2)M_1(G_1)+M_1(G_2)M_1(G_1)\\
&+ (n_2n_1^2-4m_1n_1)M_1(G_2)+8m_1m_2n_1n_2]+[[n_1^4-2n_2^2m_2]HM(G_2)\\
&+ [n_2^4-2n_2^2m_2]HM(G_1)+5n_1M_1(G_1)F(G_2)+5n_2M_1(G_2)F(G_1)\\
&+ 10n_2^2m_2n_1M_1(G_1)+10n_2n_1^2m_1M_1(G_2)+8n_2^2m_2m_1+8n_1^2m_1m_2\\
&- 8n_2m_1^2M_1(G_2)-8n_1m_2^2M_1(G_1)-4n_1^2m_1F(G_2)-4n_2^2m_2F(G_1)\\
&- 8n_1^2m_1M_2(G_2)-8n_2^2m_2M_2(G_1)+8m_1M_2(G_2)+8m_2M_2(G_1)\\
&- 8n_2n_1M_1(G_1)M_1(G_2)+4n_2M_2(G_1)M_1(G_2)+4n_1M_2(G_2)M_1(G_1)\\
&- 2F(G_1)F(G_2)-4M_2(G_1)M_2(G_2)].
\end{aligned}$$

Symmetric difference

The symmetric difference $G_1\oplus G_2$, of two simple and connected graphs G_1 and G_2 is the graph with vertex set $V(G_1)\times V(G_2)$ and $E(G_1\oplus G_2)=(u_1,u_2)(v_1,v_2)|u_1v_1\in E(G_1)$ or $u_2v_2\in E(G_2)$ but not both.

Theorem 3.12: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}
\overline{HM}(G_1 \oplus G_2) &= 4[m_1n_2^2 + m_2n_1^2 - 4m_1m_2]^2 + (n_1n_2 - 2)[(n_1n_2^2 - 8m_2n_2)M_1(G_1) \\
&+ 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2] \\
&- [[n_1^4 - 4n_2^2m_2]HM(G_2) + [n_2^4 - 4n_2^2m_2]HM(G_1) + 20n_1M_1(G_1)F(G_2) \\
&+ 20n_2M_1(G_2)F(G_1) + 10n_2^2m_2n_1M_1(G_1) + 10n_2n_1^2m_1M_1(G_2) \\
&+ 8n_2^2m_2m_1 - 16n_2m_1^2M_1(G_2) - 16n_1m_2^2M_1(G_1) - 8n_1^2m_1F(G_2) \\
&- 8n_2^2m_2F(G_1) - 16n_1^2m_1M_2(G_2) - 16n_2^2m_2M_2(G_1) + 32m_1M_2(G_2) \\
&+ 32m_2M_2(G_1) - 16n_2n_1M_1(G_1)M_1(G_2) + 16n_2M_2(G_1)M_1(G_2) \\
&+ 16n_1M_2(G_2)M_1(G_1) - 16F(G_1)F(G_2) - 32M_2(G_1)M_2(G_2)].
\end{aligned}$$

Proof. Using a similar method, as in Theorem 3.10.

Proposition 3.13: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, Then.

$$\begin{aligned}
\overline{HM}(\overline{G_1 \oplus G_2}) &= 4[m_1n_2^2 + m_2n_1^2 - 4m_1m_2](n_1n_2 - 1)^2 - 4(n_1n_2 - 1)[(n_1n_2^2 - 8m_2n_2)M_1(G_1) \\
&+ 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2] \\
&+ [n_1^4 - 4n_2^2m_2]HM(G_2) + [n_2^4 - 4n_2^2m_2]HM(G_1) + 20n_1M_1(G_1)F(G_2) \\
&+ 20n_2M_1(G_2)F(G_1) + 10n_2^2m_2n_1M_1(G_1) + 10n_2n_1^2m_1M_1(G_2) \\
&+ 8n_2^2m_2m_1 - 16n_2m_1^2M_1(G_2) - 16n_1m_2^2M_1(G_1) - 8n_1^2m_1F(G_2) \\
&- 8n_2^2m_2F(G_1) - 16n_1^2m_1M_2(G_2) - 16n_2^2m_2M_2(G_1) + 32m_1M_2(G_2) \\
&+ 32m_2M_2(G_1) - 16n_2n_1M_1(G_1)M_1(G_2) + 16n_2M_2(G_1)M_1(G_2) \\
&+ 16n_1M_2(G_2)M_1(G_1) - 16F(G_1)F(G_2) - 32M_2(G_1)M_2(G_2).
\end{aligned}$$

4. APPLICATION

TiO_2 is one of the most studied compounds in materials science. Owing to some outstanding properties it is used for instance in photocatalysis, dye-sensitized solar cells, and biomedical devices [18]. In chemical graph theory, topological indices provide an important tool to quantify the molecular structure and it is found that there is a strong correlation between the properties of chemical compounds and their molecular structure [17]. Among different topological indices, degree-based topological indices are most studied and have some important applications. In this section, hyper$-$Zagreb coindex have been investigated for titania TiO_2 nanotubes and molecular graph of nanotorus .

Corollary 4.1: The hyper-Zagreb coindex of $TiO_2[n,m]$ nanotube Fig.1. is given by $\overline{HM}(TiO_2[n,m]) = 856m^2n^2 + 1064mn^2 + 352n^2 - 732mn - 380n.$

Proof. By using Theorem 2.7. we have
$\overline{HM}(TiO_2[n,m]) = (|V(TiO_2)|-2)M_1(TiO_2[n,m]) + 4|E(TiO_2)|^2 - HM(TiO_2[n,m])$, and since $M_1(TiO_2[n,m]) = 76mn + 48n$, given in [14]. $HM(TiO_2[n,m]) = 580mn + 284n$, given in [17]. and The partitions of the vertex set and edge set $V(TiO_2), E(TiO_2)$, of $TiO_2[n,m]$ nanotubes are given in Table 1. and Table 2., respectively. We have

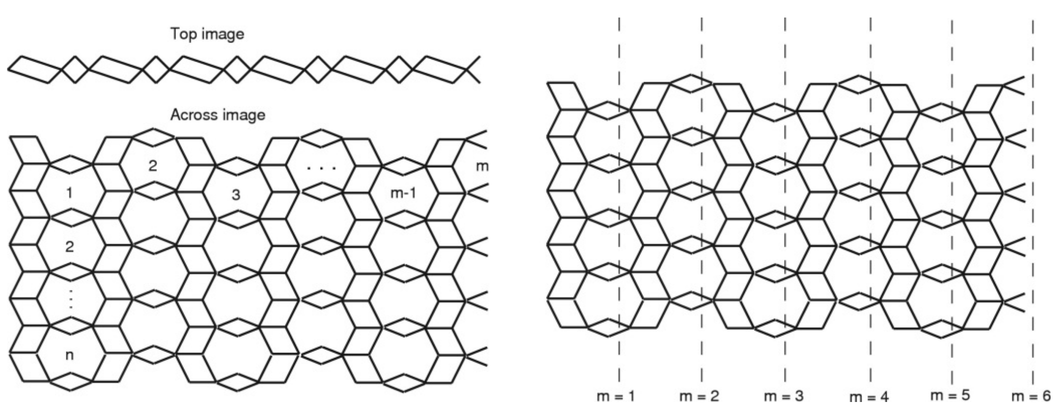

FIGURE 1. The molecular graph of $TiO_2[n,m]$ nanotube.

TABLE 1. The vertex partition of $TiO_2[n,m]$ nanotubes.

Vertex partition	v_2	v_3	v_4	v_5
Cardinality	$2mn+4n$	$2mn$	$2n$	$2mn$

TABLE 2. The edge partition of $TiO_2[n,m]$ nanotubes.

Edge partition	$E_6=E_8^*$	$E_7=E_{10}^*\cup E_{12}^*$	$E_8=E_{15}^*$	E_{12}^*	E_{10}^*
Cardinality	$6n$	$4mn+4n$	$6mn-2n$	$4mn+2n$	$2n$

$$\begin{aligned}
&\overline{HM}(TiO_2[n,m])\\
&= (\bigcup V(TiO_2[n,m])-2)M_1(TiO_2[n,m])\\
&+ 4(\bigcup E(TiO_2[n,m])^2-HM(TiO_2[n,m])\\
&= (\sum|V(TiO_2[n,m])|-2)M_1(TiO_2[n,m])\\
&+ 4(\sum|E(TiO_2[n,m])|^2-HM(TiO_2[n,m])\\
&= (6mn+6n-2)(76mn+48n)+4[|E_8^*|+|E_{10}^*\cup E_{12}^*|+|E_{15}^*|]^2\\
&- 580mn-284n\\
&= 856m^2n^2+1064mn^2+352n^2-732mn-380n.
\end{aligned}$$

Corollary 4.2: Let P_n and C_m be path and cycle graphs with n, m vertices, respectively, such that $m,n\geq 3$. Then

1. $\overline{HM}(C_n*C_m)=133n^2m^2-14m^2n-nm^4-214nm-16n$.
2. $\overline{HM}(P_n*C_m)=4m^2(4n-3)^2+2m(nm-2)(48n-61)-[16n-30+72nm-38m+4m(n-1)(2m+1)+nm^2(m^2+6)]$.
3. $\overline{HM}(P_n+C_m)=4[(n-1)+m+nm]^2+(nm-2)[4n-6+nm^2+mn^2+8nm]-[16n-38+44nm-22m+12n^2m+12m^2n+nm(m+n)^2]$.
4. $\overline{HM}(C_n+C_m)=4[(n-1)+m+nm]^2+(nm-2)[4n-6+nm^2+mn^2+8nm]-[16n-38+44nm-22m+12n^2m+12m^2n+nm(m+n)^2]$.

Corollary 4.3: Let $T = T[p,q]$ be the molecular graph of a nanotorus such that $|V(T)| = pq$, $|E(T)| = \frac{3}{2}pq$, Fig. 2. Then:

a. $\overline{HM}(T[p,q]) = 18p^2q^2 - 72pq.$

b. $\overline{HM}(P_n \times T) = 50n^2p^2q^2 - 38np^2q^2 + 4p^2q^2 - 300npq - 150pq.$

Proof. To proof (a), by using Theorem 2.7. we have

$$\overline{HM}(T[p,q]) = (|V(T[p,q])| - 2)M_1(T[p,q]) + 4|E(T[p,q])|^2 - HM(T[p,q])$$

And since $HM(T[p,q]) = 54pq$ by [13]. $M_1(T) = 9pq$ by [12]. Then

$$\overline{HM}(T[p,q]) = 9pq(pq-2) + 4[\frac{3}{2}pq]^2 - 54pq = 18p^2q^2 - 72pq.$$

To proof (b), by [13] $HM(P_n \times T) = 250npq - 186pq$, and by [12] $M_1(P_n \times T) = pq(25n - 18)$, and by using Lemma 2.1. $|E(P_n \times T)| = (n-1)pq + \frac{3}{2}npq = pq(\frac{5}{2}n - 1)$, $|V(P_n \times T)| = npq$, and by using Theorem 2.7. we get

$$\begin{aligned} &\overline{HM}(P_n \times T) \\ &= (|V(P_n \times T)| - 2)M_1(P_n \times T) + 4|E(P_n \times T)|^2 - HM(P_n \times T) \\ &= pq(npq-2)(25n-18) + 4[pq(\frac{5}{2}n-1)]^2 - 250npq - 186pq \\ &= 50n^2p^2q^2 - 38np^2q^2 + 4p^2q^2 - 300npq - 150pq. \end{aligned}$$

FIGURE 2. molecular graph of a nanotorus

5. Conclusion

The present study has investigated some of the basic mathematical properties of the Hyper-Zagreb coindex and obtained explicit formula for their values under several graph operations. and we studied the Hyper-Zagreb coindex of molecular graph of nanotorus and titania nanotubes $TiO_2[n,m]$.

Conflict of Interests

The author(s) declare that there is no conflict of interests.

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