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Research Article

The Second Hyper-Zagreb Coindex of Chemical Graphs and Some Applications

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The second hyper-Zagreb coindex is an efficient topological index that enables us to describe a molecule from its molecular graph. In this current study, we shall evaluate the second hyper-Zagreb coindex of some chemical graphs. In this study, we compute the value of the second hyper-Zagreb coindex of some chemical graph structures such as sildenafil, aspirin, and nicotine. We also present explicit formulas of the second hyper-Zagreb coindex of any graph that results from some interesting graphical operations such as tensor product, Cartesian product, composition, and strong product, and apply them on a q-multiwalled nanotorus.

1. Introduction

A graph can be identified by a corresponding numerical value, a sequence of numbers, or a special polynomial or a matrix. Special attention is directed to chemical graphs which constitute a wonderful topic in graph theory because of the abundance of applications in chemistry or in medical science [1, 2]. Topological index and coindex are invariant under graph automorphism. The computation of these numerical quantities is useful and well-proven in medical information of new drugs without resorting to chemical experiments [3, 4]. All graphs in this study are finite and simple, let G be a finite simple graph on $V(G) = n$, vertices, and $E(G) = m$, edges, and the degree of a vertex v is the number of edges event to v, denoted by $\delta_G(v)$. 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 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, we have $E(G) \bigcup E(\overline{G}) = E(K_n)$, so $\overline{m} = E(\overline{G}) = \binom{n}{2} - m$, and the degree of a vertex u in $\overline{G}$ is given by

$$\delta_{\overline{G}}(u) = n - 1 - \delta_G(u). \tag{1}$$

Gutman and Trinajestić [5] introduced the first and second Zagreb indices as follows:

$$\begin{aligned} M_1(G) &= \sum_{v \in V(G)} {\delta_G}^2(v) = \sum_{uv \in E(G)} [\delta_G(u) + \delta_G(v)], \\ M_2(G) &= \sum_{uv \in E(G)} \delta_G(u)\delta_G(v). \end{aligned} \tag{2}$$

In 2008, Došlić defined Zagreb coindices [6], which are given as follows:

$$\begin{aligned} \overline{M}_1(G) &= \sum_{uv \notin E(G)} [\delta_G(u)\delta_G(v)], \\ \overline{M}_2(G) &= \sum_{uv \notin E(G)} [\delta_G(u)\delta_G(v)]. \end{aligned} \tag{3}$$

Later in 2010, Ashrafi et al. have established the following nice formulas for the precise relationship between the first and second Zagreb indices and their coindices [7]:

$$\overline{M}_1(G) = 2m(n-1) - M_1(G),$$
$$\overline{M}_2(G) = 2m^2 - \frac{1}{2}M_1(G) - M_2(G). \quad (4)$$

In 2013, Shirdel et al. [8] introduced degree-based Zagreb indices named hyper-Zagreb index which is defined as

$$HM(G) = \sum_{uv \in E(G)} \left(\delta_G(u) + \delta_G(v)\right)^2. \quad (5)$$

In 2013, Ranjini et al. introduced and defined the third Zagreb index of a graph as [9]

$$\mathrm{Re}ZG_3(G) = \sum_{uv \in E(G)} \delta_G(u)\delta_G(v)\left[\delta_G(u) + \delta_G(v)\right]. \quad (6)$$

Furtula and Gutman in 2015 introduced the forgotten index (F-index) [10], which is defined as

$$F(G) = \sum_{v \in V(G)} {\delta_G}^3(v) = \sum_{uv \in E(G)} \left[{\delta_G}^2(u) + {\delta_G}^2(v)\right]. \quad (7)$$

In 2016, De et al. introduced forgotten coindex as follows:

$$\overline{F}(G) = \sum_{uv \notin E(G)} \left[{\delta_G}^2(u) + {\delta_G}^2(v)\right] = (n-1)M_1(G) - F(G). \quad (8)$$

In 2016, Veylaki et al. [11] introduced hyper-Zagreb coindex as follows:

$$\overline{HM}(G) = \sum_{uv \notin E(G)} \left(\delta_G(u) + \delta_G(v)\right)^2. \quad (9)$$

In 2016, Wei et al. [12] defined new version of Zagreb topological indices. It is called the hyper-Zagreb index that is defined as above. Then, the second hyper-Zagreb index of a graph G is defined as the sum of the weights $(\delta_G(u)\delta_G(v))^2$ and is equal to

$$HM_2(G) = \sum_{uv \in E(G)} \left(\delta_G(u)\delta_G(v)\right)^2. \quad (10)$$

In 2020, Alameri et al. [13, 14] defined a new degree-based of Zagreb indices named Y-index and Y-coindex as

$$Y(G) = \sum_{uv \in E(G)} \left[{\delta_G}^3(u) + {\delta_G}^3(v)\right],$$
$$\overline{Y}(G) = \sum_{uv \notin E(G)} \left[{\delta_G}^3(u) + {\delta_G}^3(v)\right], \quad (11)$$

where

$$\overline{Y}(G) = (n-1)F(G) - Y(G). \quad (12)$$

Here, we define a new version of Zagreb topological indices, based on the hyper-Zagreb index that is defined as above. It is called the second hyper-Zagreb index of a graph G and defined as the sum of the weights $(\delta_G(u)\delta_G(v))^2$, such that $uv \notin E(G)$ and is equal to

$$\overline{HM_2}(G) = \sum_{uv \notin E(G)} \left(\delta_G(u)\delta_G(v)\right)^2. \quad (13)$$

Eventhough, there are several research reports contributing to the computation of topological indices of chemical graphs. However, the studies on the computation of topological coindices of octane isomers are very limited. This study focused on one of the important topological coindices named the second hyper-Zagreb coindex. Some chemical graphs were obtained by this parameter. Moreover, the second hyper-Zagreb coindex of graph operations was computed and gave some of their applications such as a q-multiwalled nanotorus.

2. Preliminaries

This section is devoted to some preparatory results that will play a prominent role in our study.

Definition 2.1 (see [15, 16]). Suppose that G_1 and G_2 are two connected graphs, then

(i) The tensor product $G_1 \otimes G_2$ of G_1 and G_2 is the graph with $V(G_1 \otimes G_2) = V(G_1) \times V(G_2)$, and $E(G_1 \otimes G_2) = \{(u_1, u_2)(v_1, v_2) | u_1v_1 \in E(G_1), u_2v_2 \in E(G_2)\}$.

(ii) The Cartesian product $G_1 \times G_2$ of 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 $x = y$.

(iii) The composition $G_1[G_2]$ of 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 any two vertices $u = (u_1, v_1)$ 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).

(iv) The strong product $G_1 * G_2$ of G_1 and G_2 is a graph with $V(G_1 * G_2) = V(G_1) \times V(G_2)$, 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 $u_1u_2 \in E(G_1)\}$.

Lemma 2 (see [17, 18]). *Let G_1 and G_2 be graphs with $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, $|E(G_1)| = m_1$, and $|E(G_2)| = m_2$. Then,*

(i) $|V(G_1 \otimes G_2)| = |V(G_1 \times G_2)| = |V(G_1[G_2])| = |V(G_1 * G_2)| = n_1n_2$

(ii) $E(G_1 \otimes G_2)| = 2m_1m_2$

(iii) $|E(G_1 \times G_2)| = m_1n_2 + n_1m_2$

(iv) $|E(G_1[G_2])| = m_1{n_2}^2 + m_2n_1$

(v) $|E(G_1 * G_2)| = m_1n_2 + n_1m_2 + 2m_1m_2$

(vi) $\delta_{G_1 \otimes G_2}(u, v) = \delta_{G_1}(u)\delta_{G_2}(v)$

(a) $\delta_{G_1 \times G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v)$

(b) $\delta_{G_1[G_2]}(u, v) = n_2\delta_{G_1}(u) + \delta_{G_2}(v)$

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

Lemma 2.3 (see [17, 18]). *Let G_1, G_2 be two graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, then.*

(i) $M_1(G_1 \otimes G_2) = M_1(G_1)M_1(G_2)$

(ii) $M_1(G_1 \times G_2) = n_2 M_1(G_1) + n_1 M_1(G_2) + 8m_1m_2$

(iii) $M_1(G_1[G_2]) = {n_2}^3 M_1(G_1) + n_1 M_1(G_2) + 8n_2m_2m_1$

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

Lemma 2.4 (see [17, 18]). *Let G_1, G_2 be two simple graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, then*

(i) $Y(G_1 \otimes G_2) = Y(G_1)Y(G_2)$

(ii) $Y(G_1 \times G_2) = n_2 Y(G_1) + n_1 Y(G_2) + 8m_1F(G_2) + 8m_2F(G_1) + 6M_1(G_1)M_1(G_2)$

(iii) $Y(G_1[G_2]) = {n_2}^5 Y(G_1) + n_1 Y(G_2) + 8{n_2}^3 m_2 F(G_1) + 8n_2m_1F(G_2) + 6{n_2}^2 M_1(G_1)M_1(G_2)$

(iv) $Y(G_1 * G_2) = Y(G_1)[4F(G_2) + 6M_1(G_2) + 8m_2 + n_2] + 4F(G_1)[3M_1(G_2) + 2m_2] + Y(G_2)[4F(G_1) + 6M_1(G_1) + 8m_1 + n_1] + 4F(G_2)[3M_1(G_1) + 2m_1] + Y(G_1)Y(G_2) + 12F(G_1)F(G_2) + 6M_1(G_1)M_1(G_2)$

Lemma 2.5 (see [17, 18]). *Let G_1, G_2 be two simple graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, then*

(i) $HM_2(G_1 \otimes G_2) = 2HM_2(G_1)HM_2(G_2)$

(ii) $HM_2(G_1 \times G_2) = n_2 HM_2(G_1) + n_1 HM_2(G_2) + 3F(G_1)M_1(G_2) + 3F(G_2)M_1(G_1) + m_1[Y(G_2) + 4\mathrm{Re}ZG_3(G_2)] + m_2[Y(G_1) + 4\mathrm{Re}ZG_3(G_1)] + 4M_1(G_1)M_2(G_2) + 4M_1(G_2)M_2(G_1)$

(iii) $HM_2(G_1[G_2]) = {n_2}^6 HM_2(G_1) + n_1 HM_2(G_2) + {n_2}^4 m_2[Y(G_1) + 4\mathrm{Re}ZG_3(G_1)] + 4n_2m_1 \mathrm{Re}ZG_3(G_2) + 3{n_2}^2 F(G_1)M_1(G_2) + {n_2}^2 M_1(G_1)[F(G_2) + 4M_2(G_2)] + m_1{M_1}^2(G_2) + 4n_2m_2[4n_2m_2M_2(G_1) + M_1(G_1)M_1(G_2)]$

(iv) $HM_2(G_1 * G_2) = HM_2(G_2)[n_1 + 10m_1 + 10m_1(G_1) + 8m_2(G_1) + 6F(G_1) + 4ReZG_3(G_1) + Y(G_1)] + HM_2(G_2)[n_2 + 10m_2 + 10m_1(G_2) + 8m_2(G_2) + 6F(G_2) + 4ReZG_3(G_2) + Y(G_2)] + Y(G_2)[m_1 + 2M_1(G_1) + 4M_2(G_1) + F(G_1) + 2ReZG_3(G_1)]Y(G_1)[m_2 + 2M_1(G_2) + 4M_2(G_2) + F(G_2) + 2ReZG_3(G_2)] + 4ReZG_3(G_2)[m_1 + 2M_1(G_1) + 2M_2(G_1) + 2F(G_1)] + 4ReZG_3(G_1)[m_2 + 2M_1(G_2) + 2M_2(G_2) + 2F(G_2)] + F(G_2)[3M_1(G_1) + 8M_2(G_1)] + 4M_1(G_1)M_2(G_2) + 4M_1(G_2)M_2(G_1) + 2HM_2(G_1)HM_2(G_2) + 5F(G_1)F(G_2) + 6ReZG_3(G_1)ReZG_3(G_2)$

3. Main Results

In the following section, we study the second hyper-Zagreb coindex of some chemical graph structures, exactly sildenafil, aspirin, and nicotine.

Proposition 3.1. *Let G be a graph with n vertices and m edges. Then,*

$$\overline{HM}(G) = (n-2)\, M_1(G) + 4m^2 - HM(G). \tag{14}$$

Proof. For the proof (Theorem 3.2), we refer to [10]. □

Proposition 3.2. *Let G be a graph with n vertices and m edges. Then,*

$$\overline{HM_2}(G) = \frac{1}{2}\, {M_1}^2(G) - \frac{1}{2}Y(G) - HM_2(G). \tag{15}$$

Proof. By definition of the second hyper-Zagreb coindex and using a similar method, as above in Proposition 3.1, then

$$\begin{aligned} HM_2(G) + \overline{HM_2}(G) &= \left[\sum_{uv \in E(G)} + \sum_{uv \notin E(G)}\right][\delta_G(u)\delta_G(v)]^2 \\ &= \frac{1}{2}\left[\sum_{u \in V(G)}\sum_{v \in V(G)}[\delta_G(u)\delta_G(v)]^2 - \sum_{v \in V(G)}[\delta_G(v)\delta_G(v)]^2\right] \\ &= \frac{1}{2}\left[\, {M_1}^2(G) - Y(G)\right]. \end{aligned} \tag{16}$$

Sildenafil ($C_{22}H_{30}N_6O_4S$) is a drug used for pulmonary arterial hypertension. It is taken by mouth or injection into a vein (Figure 1) [19]. □

Proposition 3.3. *The second hyper-Zagreb coindex of sildenafil.*

From the graph structure of sildenafil (Figure 1), it is easy to obtain the dataset in Tables 1 and 2.

By Table 1 and definitions of the first Zagreb index and the Y-index, we have

$$\begin{aligned} M_1(\text{sildenafil}) &= (7)(1) + (14)(4) + (11)(9) + (1)(16) = 178, \\ Y(\text{sildenafil}) &= (7)(1) + (14)(16) + (11)(81) + (1)(256) = 1378. \end{aligned} \tag{17}$$

Also, by Table 2 and definition of the second hyper-Zagreb index, we have

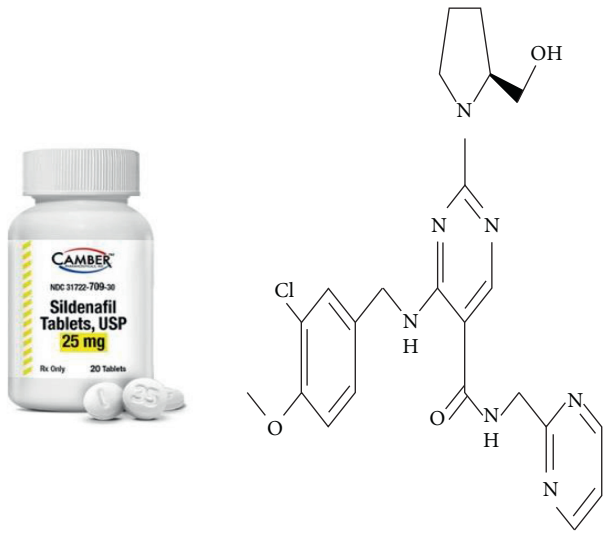

Figure 1: Graph structure of sildenafil.

Table 1: Atoms dataset of the graph structure of sildenafil.

No. of atoms	7	14	11	1
δv	1	2	3	4
$\delta^2 v$	1	4	9	16
$\delta^4 v$	1	16	81	256

Table 2: Links dataset of the graph structure of sildenafil.

No. of links	2	3	7	16	6	2
$\delta^2 u\, \delta^2 v$	4	9	16	36	81	144

$$HM_2(\text{sildenafil}) = (2)(4) + (3)(9) + (7)(16) + (16)(36) + (6)(81) + (2)(144) = 1497. \tag{18}$$

Using Proposition 3.2, we have

$$\overline{HM_2}(\text{sildenafil}) = 13656. \tag{19}$$

Aspirin ($C_9H_8O_4$) is known as acetylsalicylic acid (ASA). Aspirin has many medicinal uses as it is a drug that is used to reduce fever or inflammation, also given after a heart attack to reduce the risk of death. Aspirin is also used as a nonsteroidal anti-inflammatory drug because it has an antiplatelet effect by inhibiting its normal functioning. Also, a lot of evidence indicates that aspirin is considered a chemical agent that may limit and reduce the incidence of general cancers (Figure 2) [20, 21].

Proposition 3.4. *The second hyper-Zagreb coindex of aspirin.*

From the graph structure of aspirin (Figure 2), it is easy to obtain the dataset in Tables 2 and 3.

Also, by Table 4 and definition of the second hyper-Zagreb index, we have

$$HM_2(\text{aspirin}) = (4)(9) + (3)(16) + (4)(36) + (2)(81) = 390. \tag{20}$$

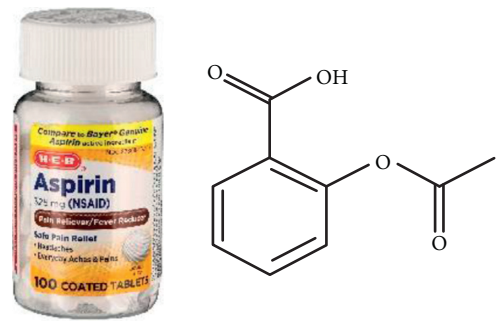

Figure 2: Graph structure of aspirin.

Table 3: Atoms dataset of the graph structure of aspirin.

No. of atoms	4	5	4
δv	1	2	3
$\delta^2 v$	1	4	9
$\delta^4 v$	1	16	81

Table 4: Links dataset of the graph structure of aspirin.

No. of links	4	3	4	2
$\delta^2 u\, \delta^2 v$	9	16	36	81

Using Proposition 3.2, we have

$$\overline{HM_2}(\text{aspirin}) = 1206. \tag{21}$$

Nicotine ($C_{10}H_{14}N_2$) is an alkaloid that is widely used as an anxiolytic. Nicotine is used as a drug to quit smoking, and if it is not used well, it can lead to addiction. Many types of research conducted on animals indicate that some inhibitors found in tobacco smoke, such as monoamine oxidase, may enhance some of the addictive properties of nicotine (Figure 3) [21, 22]. Any unexplained terminology is standard, typically as in [22–24].

By Table 3 and definitions of the first Zagreb index and the Y-index, we have

$$M_1(\text{aspirin}) = (4)(1) + (5)(4) + (4)(9) = 60, \quad Y(\text{aspirin}) = (4)(1) + (5)(16) + (4)(81) = 408. \tag{22}$$

Proposition 3.5. *The second hyper-Zagreb coindex of nicotine.*

From the graph structure of nicotine (Figure 3), it is easy to obtain the dataset in Tables 5 and 6.

By Table 5 and definitions of the first Zagreb index and the Y-index, we have

$$M_1(\text{nicotine}) = (1)(1) + (8)(4) + (3)(9) = 60, \quad Y(\text{nicotine}) = (1)(1) + (8)(16) + (3)(81) = 372. \tag{23}$$

Also, by Table 6 and definition of the second hyper-Zagreb index, we have

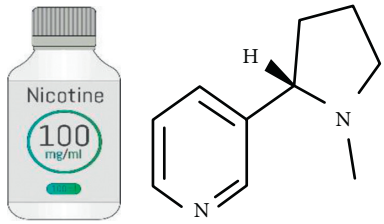

Figure 3: Graph structure of nicotine.

Table 5: Atoms dataset of the graph structure of nicotine.

No. of atoms	1	8	3
δv	1	2	3
$\delta^2 v$	1	4	9
$\delta^4 v$	1	16	81

Table 6: Links dataset of the graph structure of nicotine.

No. of links	1	6	4	2
$\delta^2 u\, \delta^2 v$	9	16	36	81

$$HM_2(\text{nicotine}) = (1)(9) + (6)(16) + (4)(36) + (2)(81) = 483. \tag{24}$$

Using Proposition 3.2, we have

$$\overline{HM_2}(\text{nicotine}) = 1131. \tag{25}$$

4. Applications

In the following section, we provide the exact value of the second hyper-Zagreb coindex of graphs that are arisen from mathematical operations such as the tensor product $G_1 \otimes G_2$, the Cartesian product $G_1 \times G_2$, the composition $G_1[G_2]$, and the strong product $G_1 * G_2$. Also, we apply this coindex on a q-multiwalled nanotorus.

Theorem 4.1. *The second hyper-Zagreb coindex of $G_1 \times G_2$ is given by*

$$\begin{aligned}\overline{HM_2}(G_1 \times G_2) = {} & \frac{1}{2}[n_2 M_1(G_1) + n_1 M_1(G_2) + 8m_1 m_2]^2 \\ & - \frac{1}{2}[n_2 Y(G_1) + n_1 Y(G_2) + 8m_1 F(G_2) \\ & + 8m_2 F(G_1) + 6M_1(G_1) M_1(G_2)] \\ & - [n_2 HM_2(G_1) + n_1 HM_2(G_2) \\ & + 3F(G_1) M_1(G_2) + 3F(G_2) M_1(G_1) \\ & + m_1[Y(G_2) + 4\mathrm{Re}ZG_3(G_2)] \\ & + m_2[Y(G_1) + 4\mathrm{Re}ZG_3(G_1)] + 4M_1 \\ & \cdot (G_1) M_2(G_2) + 4M_1(G_2) M_2(G_1)].\end{aligned} \tag{26}$$

Proof. We have $\overline{HM_2}(G) = 1/2{M_1}^2(G) - 1/2Y(G) - HM_2(G)$, given in Proposition 3.2, and by replacing each G by $G_1 \times G_2$, which yields $\overline{HM_2}(G_1 \times G_2) = 1/2{M_1}^2(G_1 \times G_2) - 1/2Y(G_1 \times G_2) - HM_2(G_1 \times G_2)$, and by using (Lemma 2.2–Lemma 2.4), we obtain the required.

All proofs in Theorems 4.2–4.4 are given as Theorem 4.1. □

Theorem 4.2. *The second hyper-Zagreb coindex of $G_1 * G_2$ is given by*

$$\begin{aligned}\overline{HM_2}(G_1 * G_2) = {} & \frac{1}{2}[(n_2 + 6m_2) M_1(G_1) + 8m_2 m_1 (6m_1 + n_1) M_1(G_2) + 2M_1(G_1) M_1(G_2)]^2 \\ & - \frac{1}{2}[Y(G_1)[4F(G_2) + 6M_1(G_2) + 8m_2 + n_2] + 4F(G_1)[3M_1(G_2) + 2m_2] \\ & + Y(G_2)[4F(G_1) + 6M_1(G_1) + 8m_1 + n_1] + 4F(G_2)[3M_1(G_1) + 2m_1] \\ & + Y(G_1) Y(G_2) + 12F(G_1) F(G_2) + 6M_1(G_1) M_1(G_2)] - HM_2(G_2) \\ & \cdot [n_1 + 10m_1 + 10M_1(G_1) + 8M_2(G_1) + 6F(G_1) + 4ReZG_3(G_1) + Y(G_1)] \\ & + HM_2(G_1)[n_2 + 10m_2 + 10M_1(G_2) + 8M_2(G_2) + 6F(G_2) + 4ReZG_3(G_2) + Y(G_2)] \\ & + Y(G_2)[m_1 + 2M_1(G_1) + 4M_2(G_1) + F(G_1) + 2ReZG_3(G_1)] + Y(G_1)[m_2 + 2M_1(G_2) + 4M_2(G_2) \\ & + F(G_2) + 2ReZG_3(G_2)] + 4ReZG_3(G_2)[m_1 + 2M_1(G_1) + 2M_2(G_1) + 2F(G_1)]. \\ & + 4ReZG_3(G_1)[m_2 + 2M_1(G_2) + 2M_2(G_2) + 2F(G_2)] + F(G_2)[3M_1(G_1) + 8M_2(G_1)] \\ & + F(G_1)[3M_1(G_2) + 8M_2(G_2)].\end{aligned} \tag{27}$$

Theorem 4.3. *The second hyper-Zagreb coindex of $G_1 \otimes G_2$ is given by*

$$\begin{aligned}\overline{HM}_2(G_1 \otimes G_2) &= \frac{1}{2}[M_1(G_1)M_1(G_2)]^2 \\ &\quad - \frac{1}{2}[Y(G_1)Y(G_2)] \\ &\quad - [2HM_2(G_1)HM_2(G_2)].\end{aligned} \tag{28}$$

Theorem 4.4. *The second hyper-Zagreb coindex of $G_1[G_2]$ is given by*

Proof. $\overline{HM_2}(G_1[G_2]) = 1/2[n_2^3 M_1(G_1) + n_1 M_1(G_2) + 8\, n_2 m_2 m_1 Y(G_1[G_2]) = n_2^5 Y(G_1) + n_1 Y(G_2) + 8n_2^3 m_2 F(G_1) + 8n_2 m_1 F(G_2) + 6n_2^2 M_1 (G_1)M_1(G_2)]^2 + -1/2[n_2^5 Y(G_1) + n_1 Y(G_2) + 8n_2^3 m_2 F(G_1) + 8n_2 m_1 F(G_2) + 6n_2^2 M_1(G_1)M_1(G_2)] - [n_2{}^6 HM_2(G_1) + n_1 HM_2(G_2) + n_2{}^4 m_2[Y(G_1) + 4\mathrm{Re}ZG_3(G_1)] + 4n_2 m_1 \mathrm{Re}ZG_3(G_2) + 3n_2{}^2 F(G_1)M_1(G_2) + n_2{}^2 M_1(G_1)[F(G_2) + 4M_2(G_2)] + m_1 M_1{}^2(G_2) + 4n_2 m_2[4n_2 m_2 M_2(G_1) + M_1(G_1)M_1(G_2)]]$.

In [19, 25–27], authors computed some topological indices of molecular graph of a nanotorus (Figure 4). In this section, we compute the second hyper-Zagreb coindex of a molecular graph of a nanotorus. □

Corollary 4.5. *Let $T = T[p; q]$ be the molecular graph of a nanotorus. Then, the first Zagreb index of a q-multiwalled nanotorus is $M_1(P_n \times T) = pq(25n - 18)$.*

Proof. The proof of the above corollary is given by Gao et al. in [3]. Obviously,

$$\begin{aligned}|V(G_1)| &= |V(P_n)| = n, \\ |E(G_1)| &= |E(P_n)| = n - 1, \\ |V(G_2)| &= |V(T)| = pq, \\ |E(G_2)| &= |E(T)| = \left(\frac{3}{2}\right)pq, \\ |M_1(G_1)| &= |M_1(P_n)| = (4n - 6), \\ |M_1(G_2)| &= |M_1(T)| = 9pq.\end{aligned} \tag{29}$$

□

Corollary 4.6. *Let $T = T[p; q]$ be the molecular graph of a nanotorus. Then, the Y-index of a q-multiwalled nanotorus is*

$$Y(P_n \times T) = pq(625n - 738). \tag{30}$$

Proof. We have by Lemma 4.2,

$$\begin{aligned}Y(G_1 \times G_2) &= n_2 Y(G_1) + n_1 Y(G_2) + 8m_1 F(G_2) \\ &\quad + 8m_2 F(G_1) + 6M_1(G_1)M_1(G_2).\end{aligned} \tag{31}$$

Then,

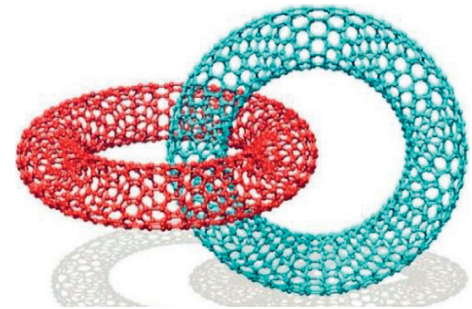

Figure 4: The molecular graph of a nanotorus.

$$\begin{aligned}Y(P_n \times T) &= (pq)Y(P_n) + nY(T) + 8(n-1)F(T) \\ &\quad + 8\left(\frac{3}{2}\right)pqF(P_n) + 6M_1(P_n)M_1(T).\end{aligned} \tag{32}$$

Therefore,

$$\begin{aligned}Y(P_n \times T) &= (pq)(16n - 30) + n(81pq) + 8(n-1)(27pq) \\ &\quad + 12pq(8n - 14) + 6(4n - 6)(9pq) \\ &= pq(625n - 738).\end{aligned} \tag{33}$$

□

Corollary 4.7. *Let $T = T[p; q]$ be the molecular graph of a nanotorus. Then, the second hyper-Zagreb index of a q-multiwalled nanotorus is*

$$HM_2(P_n \times T) = \left(\frac{1}{2}\right)pq(2561n - 3632). \tag{34}$$

Proof. We have by Lemma 2.5,

$$\begin{aligned}HM_2(G_1 \times G_2) &= n_2 HM_2(G_1) + n_1 HM_2(G_2) \\ &\quad + 3F(G_1)M_1(G_2) + 3F(G_2)M_1(G_1) \\ &\quad + m_1[Y(G_2) + 4\mathrm{Re}ZG_3(G_2)] \\ &\quad + m_2[Y(G_1) + 4\mathrm{Re}ZG_3(G_1)] \\ &\quad + 4M_1(G_1)M_2(G_2) + 4M_1(G_2)M_2(G_1).\end{aligned} \tag{35}$$

As proof in Corollary 4.6, we have

$$HM_2(P_n \times T) = \left(\frac{1}{2}\right)pq(2561n - 3632), \tag{36}$$

where

$$|HM_2(P_n)| = (16n - 40), \quad |HM_2(T)| = \left(\frac{243}{2}\right)pq. \tag{37}$$

Now, we apply the second hyper-Zagreb coindex on a q-multiwalled nanotorus using Cartesian product operation. □

Corollary 4.8. *Let $T = T[p; q]$ be the molecular graph of a nanotorus. Then, the second hyper-Zagreb coindex of a q-multiwalled nanotorus is*

$$\overline{HM_2}(P_n \times T) = \left(\frac{1}{2}\right) pq\left[pq(25n-18)^2 - 3186n + 4370\right]. \tag{38}$$

Proof. We have by Proposition 3.2,

$$\overline{HM_2}(G) = \frac{1}{2}\, {M_1}^2(G) - \frac{1}{2} Y(G) - HM_2(G). \tag{39}$$

Then,

$$\overline{HM_2}(P_n \times T) = \frac{1}{2}\, {M_1}^2(P_n \times T) - \frac{1}{2} Y(G) - HM_2(P_n \times T). \tag{40}$$

By using Corollaries 4.5–4.7, we obtain

$$\overline{HM_2}(P_n \times T) = \left(\frac{1}{2}\right) pq\left[pq(25n-18)^2 - 3186n + 4370\right]. \tag{41}$$

□

5. Conclusion

In this study, we obtained the value of the second hyper-Zagreb coindex of some chemical graphs, and we computed some explicit formulas for their numbers under several graph operations. Also, we applied the second hyper-Zagreb coindex on a q-multiwalled nanotorus. The results of this work may be used as a predictor, especially in the chemical graph theory. For example, in quantitative structure-activity relationships (QSAR) modelling, the predictors consist of theoretical molecular descriptors of chemicals.

Data Availability

No data were used to support this study, except for the references that were mentioned.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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