

# The second Hyper-Zagreb index of complement graphs and its applications of some Nano Structures

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## Abstract

In chemical graph theory, a topological descriptor is a numerical quantity that is based on the chemical structure of underlying chemical compound. Topological indices play an important role in chemical graph theory especially in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR). In this paper, we present explicit formulae for some basic mathematical operations for the second hyper-Zagreb index of complement graph containing the join  $G_1 + G_2$ , tensor product  $G_1 \otimes G_2$ , Cartesian product  $G_1 \times G_2$ , composition  $G_1 \circ G_2$ , strong product  $G_1 * G_2$ , disjunction  $G_1 \vee G_2$  and symmetric difference  $G_1 \oplus G_2$ . Moreover, we studied the second hyper-Zagreb index for some certain important physicochemical structures such as molecular complement graphs of V-Phenylenic Nanotube  $VPHX[q, p]$ , V-Phenylenic Nanotorus  $VPHY[m, n]$  and Titania Nanotubes  $TiO_2$ .

*Keywords:* Zagreb index, Hyper-Zagreb index, Y-index, Second Hyper-Zagreb index, Forgotten index, graph operation, Titania Nanotubes, V-Phenylenic Nanotube  $VPHX[q, p]$ , V-Phenylenic Nanotorus  $VPHY[m, n]$ , complement graph.

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## 1. Introduction

A graph can be recognized by a numeric value which represent the whole graph. Topological indices are numerical quantity which are used to correlate the physico-chemical properties of a molecule with its structure such as boiling point, stability, strain energy etc. There are a wide range of topological descriptors which based on degree-based, distance-based, eigenvalue-based, matching-based and mixed-based. The topological indices which based on degree-based play a vital in chemical sciences and computing these topological indices is one of the recent areas of research in chemical graph theory. In our study, we have computed the degree-based topological indices of some graph operations and some nanostructure. All graphs in this paper are finite and simple, let  $G$  be a finite simple graph on  $V(G) = n$ , vertices and  $E(G) = m$ , edges, the degree of a vertex  $v$  is the number of edges incident to  $v$ , denoted by  $\delta_G(v)$ . The first and second Zagreb indices have been introduced by Gutman and Trinajstić in 1972 [1]. They are respectively defined as:

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

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

The first and second Zagreb coindices have been introduced by A.R. Ashrafi, T. Došlić, and A. Hamzeh in 2010 [2]. They are respectively defined as:

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

In 2013, Shirdel et al. [3] introduced degree-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, M. Veylaki et al. [4] introduced degree-based of Zagreb coindex 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) [5]. which defined as:

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

Furtula et al. in (2015) defined forgotten coindex (F-coindex)[6] as the following:

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

Ranjini et al. [7] defined the redefined first, second and third Zagreb indices for a graph  $G$  and these are manifested as:

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{\delta(u) + \delta(v)}{\delta(u)\delta(v)}, \quad ReZG_2(G) = \sum_{uv \in E(G)} \frac{\delta(u)\delta(v)}{\delta(u) + \delta(v)},$$

$$ReZG_3(G) = \sum_{uv \in E(G)} (\delta_G(u) \delta_G(v))(\delta_G(u) + \delta_G(v)),$$

In 2020, Alameri et al. [8, 9] presented new degree-based of Zagreb index and coindex denoted by (Y-index, Y-coindex) and defined respectively as:

$$Y(G) = \sum_{u \in V(G)} \delta_G^4(u) = \sum_{uv \in E(G)} [\delta_G^3(u) + \delta_G^3(v)],$$

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

In 2016, Wei Gao et al [10] defined the second Hyper-Zagreb index of a graph  $G$ , which is defined as:

$$HM_2(G) = \sum_{uv \in E(G)} (\delta_G(u) \delta_G(v))^2,$$

Therefore, Wei Gao et al. [10] in (2016) computed the second Hyper-Zagreb index  $HM_2(G)$  of Carbon Nanocones  $CNC_k[n]$ . M. Farahani et al. [11] studied the second Hyper-Zagreb index of Molecular graphs V-Phenylenic Nanotubes and V-Phenylenic Nanotorus. A. Modabish et al. [12] in (2021) computed the second Hyper-Zagreb index of some special graph and graph operation. Here we continue this line of research by exploring the behavior of the second Hyper-Zagreb index under several important operations such as the tensor product  $\overline{G_1} \otimes \overline{G_2}$ , join  $G_1 + G_2$  and  $\overline{G_1} + \overline{G_2}$ , strong product  $G_1 * G_2$ , disjunction  $\overline{G_1} \vee \overline{G_2}$  and symmetric difference  $\overline{G_1} \oplus \overline{G_2}$ . The results are applied on some molecular complement graphs such as of V-Phenylenic Nanotube  $VPHX[q, p]$ , V-Phenylenic Nanotorus  $VPHY[m, n]$  and Titania Nanotubes  $TiO_2$ . Any unexplained terminology is standard, typically as in [10, 11, 13, 14, 15, 16, 17, 18].

## 2. Preliminaries

**Definition 2.1**[25] *The complement graph of a graph  $G$  denoted by  $\overline{G}$ , is a 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,  $uv \in E(\overline{G})$ ,  $\iff uv \notin E(G)$ . 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  $\delta_{\overline{G}}(u) = (n - 1) - \delta_G(u)$ .*

**Theorem 2.2** [11, 19] *The first and second Zagreb and Hyper-Zagreb indices of the V-Phenylenic Nanotubes  $VPHX[q, p](\forall q, p \in \mathbb{N} - \{1\})$  (Fig 1.) are given by,*

$$\begin{aligned} M_1(VPHX[q, p]) &= 54pq - 10q, \\ M_2(VPHX[q, p]) &= 81pq + 3q, \\ HM(VPHX[q, p]) &= 4q(81p - 20), \\ HM_2(VPHX[q, p]) &= 9q(81p - 29). \end{aligned}$$

**Theorem 2.3** [11, 19] *The Zagreb and Hyper-Zagreb indices of the V-Phenylenic Nanotorus  $VPHY[m, n](\forall m, n \in \mathbb{N} - \{1\})$  (Fig 3.) are given by,*

$$\begin{aligned} M_1(VPHY[m, n]) &= 54mn, \\ M_2(VPHY[m, n]) &= 81mn, \\ HM(VPHY[m, n]) &= 324mn, \\ HM_2(VPHY[m, n]) &= 729mn. \end{aligned}$$

## 3. Discussion and Main Results

In this section, we study the second Hyper-Zagreb index of various complement graph operations and compute  $HM_2$  for some certain important Nano-Structures such as molecular complement graphs of V-Phenylenic Nanotube  $VPHX[q, p]$ , V-Phenylenic Nanotorus  $VPHY[m, n]$  and Titania Nanotubes  $TiO_2$ .

### 3.1. Second Hyper-Zagreb index of complement graph binary operations

**Theorem 3.1.1** Let  $G$  be a graph with  $n$  vertices and  $m$  edges. Then,

$$\begin{aligned} HM_2(\overline{G}) &= m(n-1)^4 - 2(n-1)^3 M_1(G) + (n-1)^2 F(G) + 4(n-1)^2 M_2(G) \\ &\quad - 2(n-1) M_1(G) F(G) + HM_2(G). \end{aligned}$$

**Proof.** By definition of the second Hyper-Zagreb index, we have

$$\begin{aligned} HM_2(\overline{G}) &= \sum_{uv \notin E(G)} [\delta_{\overline{G}}(u) \delta_{\overline{G}}(v)]^2 \\ &= \sum_{uv \in E(G)} [(n-1) - \delta_G(u)]^2 [(n-1) - \delta_G(v)]^2 \\ &= \sum_{uv \in E(G)} [[(n-1)^2 - 2(n-1)\delta_G(u) + \delta_G^2(u)][(n-1)^2 - 2(n-1)\delta_G(v) + \delta_G^2(v)]] \\ &= \sum_{uv \in E(G)} [(n-1)^2 [(n-1)^2 - 2(n-1)\delta_G(v) + \delta_G^2(v)] \\ &\quad - 2(n-1)\delta_G(u)[(n-1)^2 - 2(n-1)\delta_G(v) + \delta_G^2(v)] \\ &\quad + \delta_G^2(u)[(n-1)^2 - 2(n-1)\delta_G(v) + \delta_G^2(v)]] \\ &= \sum_{uv \in E(G)} [(n-1)^4 - 2(n-1)^3 \delta_G(v) + (n-1)^2 \delta_G^2(v) - 2(n-1)^3 \delta_G(u) \\ &\quad + 4(n-1)^2 \delta_G(u) \delta_G(v) - 2(n-1) \delta_G(u) \delta_G^2(v) + (n-1)^2 \delta_G^2(u) \\ &\quad - 2(n-1) \delta_G^2(u) \delta_G(v) + \delta_G^2(u) \delta_G^2(v)] \\ &= \sum_{uv \in E(G)} [(n-1)^4 - 2(n-1)^3 \delta_G(v) - 2(n-1)^3 \delta_G(u) + (n-1)^2 \delta_G^2(v) \\ &\quad + (n-1)^2 \delta_G^2(u) + 4(n-1)^2 \delta_G(u) \delta_G(v) - 2(n-1) \delta_G(u) \delta_G^2(v) \\ &\quad - 2(n-1) \delta_G^2(u) \delta_G(v) + \delta_G^2(u) \delta_G^2(v)] \\ &= (n-1)^4 \sum_{uv \in E(G)} 1 - 2(n-1)^3 \sum_{uv \in E(G)} [\delta_G(v) + \delta_G(u)] \\ &\quad + (n-1)^2 \sum_{uv \in E(G)} [\delta_G^2(v) + \delta_G^2(u)] + 4(n-1)^2 \sum_{uv \in E(G)} \delta_G(u) \delta_G(v) \\ &\quad - 2(n-1) \sum_{uv \in E(G)} [\delta_G(u) \delta_G^2(v) + \delta_G^2(u) \delta_G(v)] + \sum_{uv \in E(G)} \delta_G^2(u) \delta_G^2(v) \\ &= m(n-1)^4 - 2(n-1)^3 M_1(G) + (n-1)^2 F(G) + 4(n-1)^2 M_2(G) \\ &\quad - 2(n-1) M_1(G) F(G) + HM_2(G). \end{aligned}$$

<sup>40</sup> **Definition 3.1.2** [20, 21] *The tensor product  $G_1 \otimes G_2$  of two graphs  $G_1$  and  $G_2$  is the graph with vertex set  $V(G_1) \times V(G_2)$  and  $E(G_1 \otimes G_2) = (u_1, u_2)(v_1, v_2) | u_1 v_1 \in E(G_1)$  and  $u_2 v_2 \in E(G_2)$ , such that  $|V(G_1 \otimes G_2)| = n_1 n_2$ ,  $|E(G_1 \otimes G_2)| = 2m_1 m_2$  and  $\delta_{G_1 \otimes G_2}(u, v) = \delta_{G_1}(u) \delta_{G_2}(v)$ .*

**Theorem 3.1.3** The second Hyper-Zagreb index of complement  $G_1 \otimes G_2$  is given by:

$$\begin{aligned} HM_2(\overline{G_1 \otimes G_2}) &= 2m_1m_2(n_1n_2 - 1)^4 - 2(n_1n_2 - 1)^3M_1(G_1)M_1(G_2) \\ &+ (n_1n_2 - 1)^2F(G_1)F(G_2) + 8(n_1n_2 - 1)^2M_2(G_1)M_2(G_2) \\ &- 2(n_1n_2 - 1)M_1(G_1)M_1(G_2)F(G_1)F(G_2) + 2HM_2(G_1)HM_2(G_2). \end{aligned}$$

45 **Proof.** By (Theorem 3.1.1) we have

$$\begin{aligned} HM_2(\overline{G}) &= m(n-1)^4 - 2(n-1)^3M_1(G) + (n-1)^2F(G) + 4(n-1)^2M_2(G) \\ &- 2(n-1)M_1(G)F(G) + HM_2(G). \end{aligned}$$

And  $M_1(G_1 \otimes G_2) = M_1(G_1)M_1(G_2)$ ,  $M_2(G_1 \otimes G_2) = 2M_2(G_1)M_2(G_2)$  given in [22].  $F(G_1 \otimes G_2) = F(G_1)F(G_2)$  given in [23].  $HM_2(G_1 \otimes G_2) = 2HM_2(G_1)HM_2(G_2)$  given in [12]. and since  $|E(G_1 \otimes G_2)| = 2m_1m_2$ ,  $|V(G_1 \otimes G_2)| = n_1n_2$ . Then,

$$\begin{aligned} HM_2(\overline{G_1 \otimes G_2}) &= |E(G_1 \otimes G_2)|(|V(G_1 \otimes G_2)| - 1)^4 - 2(|V(G_1 \otimes G_2)| - 1)^3M_1(G_1 \otimes G_2) \\ &+ (|V(G_1 \otimes G_2)| - 1)^2F(G_1 \otimes G_2) + 4(|V(G_1 \otimes G_2)| - 1)^2M_2(G_1 \otimes G_2) \\ &- 2(|V(G_1 \otimes G_2)| - 1)M_1(G_1 \otimes G_2)F(G_1 \otimes G_2) + HM_2(G_1 \otimes G_2) \\ &= 2m_1m_2(n_1n_2 - 1)^4 - 2(n_1n_2 - 1)^3M_1(G_1)M_1(G_2) \\ &+ (n_1n_2 - 1)^2F(G_1)F(G_2) + 8(n_1n_2 - 1)^2M_2(G_1)M_2(G_2) \\ &- 2(n_1n_2 - 1)M_1(G_1)M_1(G_2)F(G_1)F(G_2) + 2HM_2(G_1)HM_2(G_2). \end{aligned}$$

**Definition 3.1.4** [20, 21] The join  $G_1+G_2$  of two 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  $E(G_1) \cup E(G_2) \cup \{uv | u \in V(G_1), v \in V(G_2)\}$ , such that  $|V(G_1+G_2)| = n_1 + n_2$ ,  $|E(G_1+G_2)| = m_1 + m_2 + n_1n_2$  and

$$\delta_{G_1+G_2}(a) = \begin{cases} \delta_{G_1}(a) + n_2 & a \in V(G_1) \\ \delta_{G_2}(a) + n_1 & a \in V(G_2) \end{cases}.$$

**Theorem 3.1.5** [25] The second Zagreb index of  $G_1 + G_2$  is given by:

$$\begin{aligned} M_2(G_1 + G_2) &= M_2(G_1) + M_2(G_2) + n_2M_1(G_1) + n_1M_1(G_2) + n_2^2m_1 + n_1^2m_2 \\ &+ 4m_1m_2 + 2m_1n_1n_2 + 2m_2n_2n_1 + n_1^2n_2^2. \end{aligned}$$

50 **Theorem 3.1.6** The second Hyper-Zagreb index of  $G_1 + G_2$  is given by:

$$\begin{aligned} HM_2(G_1 + G_2) &= n_2^2F(G_1) + n_1^2F(G_2) + 4n_2^2M_2(G_1) + 4n_1^2M_2(G_2) \\ &+ 2n_2^3M_1(G_1) + 2n_1^3M_1(G_2) + n_2^4m_1 + n_1^4m_2 + n_1^3n_2^3 \\ &+ [4n_1m_2 + n_1^2n_2]M_1(G_1) + [4n_2m_1 + n_1n_2^2]M_1(G_2) \\ &+ 4n_1^2n_2^2[m_1 + m_2] + 16n_1n_2m_1m_2 + M_1(G_1)M_1(G_2) \\ &+ 2n_2M_1(G_1)F(G_1) + 2n_1M_1(G_2)F(G_2) + HM_2(G_1) + HM_2(G_2). \end{aligned}$$

**Proof.** By definitions of the second Hyper-Zagreb index, we have

$$\begin{aligned}
HM_2(G_1 + G_2) &= \sum_{uv \in E(G_1 + G_2)} [\delta_{G_1 + G_2}^2(u) \delta_{G_1 + G_2}^2(v)] \\
&= \sum_{uv \in E(G_1)} [\delta_{G_1 + G_2}^2(u) \delta_{G_1 + G_2}^2(v)] + \sum_{uv \in E(G_2)} [\delta_{G_1 + G_2}^2(u) \delta_{G_1 + G_2}^2(v)] \\
&+ \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1 + G_2}^2(u) \delta_{G_1 + G_2}^2(v)] \\
&= \sum_{uv \in E(G_1)} [(\delta_{G_1}(u) + n_2)^2 (\delta_{G_1}(v) + n_2)^2] \\
&+ \sum_{uv \in E(G_2)} [(\delta_{G_2}(u) + n_1)^2 (\delta_{G_2}(v) + n_1)^2] \\
&+ \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [(\delta_{G_1}(u) + n_2)^2 (\delta_{G_2}(v) + n_1)^2] \\
&= \sum_{uv \in E(G_1)} [(\delta_{G_1}^2(u) + 2n_2 \delta_{G_1}(u) + n_2^2) (\delta_{G_1}^2(v) + 2n_2 \delta_{G_1}(v) + n_2^2)] \\
&+ \sum_{uv \in E(G_2)} [(\delta_{G_2}^2(u) + 2n_1 \delta_{G_2}(u) + n_1^2) (\delta_{G_2}^2(v) + 2n_1 \delta_{G_2}(v) + n_1^2)] \\
&+ \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [(\delta_{G_1}^2(u) + 2n_2 \delta_{G_1}(u) + n_2^2) (\delta_{G_2}^2(v) + 2n_1 \delta_{G_2}(v) + n_1^2)] \\
&= \sum_{uv \in E(G_1)} [\delta_{G_1}^2(u) \delta_{G_1}^2(v) + 2n_2 \delta_{G_1}^2(u) \delta_{G_1}(v) + n_2^2 \delta_{G_1}^2(u) + 2n_2 \delta_{G_1}(u) \delta_{G_1}^2(v) \\
&+ 4n_2^2 \delta_{G_1}(u) \delta_{G_1}(v) + 2n_2^3 \delta_{G_1}(u) + n_2^2 \delta_{G_1}^2(v) + 2n_2^3 \delta_{G_1}(v) + n_2^4] \\
&+ \sum_{uv \in E(G_2)} [\delta_{G_2}^2(u) \delta_{G_2}^2(v) + 2n_1 \delta_{G_2}^2(u) \delta_{G_2}(v) + n_1^2 \delta_{G_2}^2(u) + 2n_1 \delta_{G_2}(u) \delta_{G_2}^2(v) \\
&+ 4n_1^2 \delta_{G_2}(u) \delta_{G_2}(v) + 2n_1^3 \delta_{G_2}(u) + n_1^2 \delta_{G_2}^2(v) + 2n_1^3 \delta_{G_2}(v) + n_1^4] \\
&+ \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}^2(u) \delta_{G_2}^2(v) + 2n_1 \delta_{G_1}^2(u) \delta_{G_2}(v) + n_1^2 \delta_{G_1}^2(u) \\
&+ 2n_2 \delta_{G_1}(u) \delta_{G_2}^2(v) + 4n_1 n_2 \delta_{G_1}(u) \delta_{G_2}(v) + 2n_1^2 n_2 \delta_{G_1}(u) + n_2^2 \delta_{G_2}^2(v) \\
&+ 2n_1 n_2^2 \delta_{G_2}(v) + n_1^2 n_2^2]
\end{aligned}$$

Step 1

$$\begin{aligned}
\sum_{uv \in E(G_1)} [...] &= \sum_{uv \in E(G_1)} [\delta_{G_1}^2(u) \delta_{G_1}^2(v)] + 2n_2 \sum_{uv \in E(G_1)} [\delta_{G_1}^2(u) \delta_{G_1}(v) + \delta_{G_1}(u) \delta_{G_1}^2(v)] \\
&+ n_2^2 \sum_{uv \in E(G_1)} [\delta_{G_1}^2(u) + \delta_{G_1}^2(v)] + 4n_2^2 \sum_{uv \in E(G_1)} [\delta_{G_1}(u) \delta_{G_1}(v)] \\
&+ 2n_2^3 \sum_{uv \in E(G_1)} [\delta_{G_1}(u) + \delta_{G_1}(v)] + n_2^4 \sum_{uv \in E(G_1)} (1) \\
&= HM_2(G_1) + 2n_2 M_1(G_1) F(G_1) + n_2^2 F(G_1) + 4n_2^2 M_2(G_1) \\
&+ 2n_2^3 M_1(G_1) + n_2^4 m_1.
\end{aligned}$$

Step 2

$$\begin{aligned}
\sum_{uv \in E(G_2)} [\dots] &= \sum_{uv \in E(G_2)} [\delta_{G_2}^2(u)\delta_{G_2}^2(v)] + 2n_1 \sum_{uv \in E(G_2)} [\delta_{G_2}^2(u)\delta_{G_2}(v) + \delta_{G_2}(u)\delta_{G_2}^2(v)] \\
&+ n_1^2 \sum_{uv \in E(G_2)} [\delta_{G_2}^2(u) + \delta_{G_2}^2(v)] + 4n_1^2 \sum_{uv \in E(G_2)} [\delta_{G_2}(u)\delta_{G_2}(v)] \\
&+ 2n_1^3 \sum_{uv \in E(G_2)} [\delta_{G_2}(u) + \delta_{G_2}(v)] + n_1^4 \sum_{uv \in E(G_2)} (1) \\
&= HM_2(G_2) + 2n_1M_1(G_2)F(G_2) + n_1^2F(G_2) + 4n_1^2M_2(G_2) \\
&+ 2n_1^3M_1(G_2) + n_1^4m_2.
\end{aligned}$$

55 Step 3

$$\begin{aligned}
\sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\dots] &= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}^2(u)\delta_{G_2}^2(v)] + 2n_1 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}^2(u)\delta_{G_2}(v)] \\
&+ n_1^2 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_1}^2(u) + 2n_2 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}(u)\delta_{G_2}^2(v)] \\
&+ 4n_1n_2 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}(u)\delta_{G_2}(v)] + 2n_1^2n_2 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_1}(u) \\
&+ n_2^2 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_2}^2(v) + 2n_1n_2^2 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_2}(v) \\
&+ n_1^2n_2^2 \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} (1) \\
&= M_1(G_1)M_1(G_2) + 4n_1m_2M_1(G_1) + n_1^2n_2M_1(G_1) + 4n_2m_1M_1(G_2) \\
&+ 16n_1n_2m_1m_2 + 4m_1n_1^2n_2^2 + n_1n_2^2M_1(G_2) + 4m_2n_1^2n_2^2 + n_1^3n_2^3.
\end{aligned}$$

It is easy to see that the summation of step 1, step 2 and step 3 complete the proof.  $\square$

**Theorem 3.1.7** The second Hyper-Zagreb index of complement  $G_1 + G_2$  is given by:

$$\begin{aligned}
HM_2(\overline{G_1 + G_2}) &= (m_1 + m_2 + n_1n_2)(n_1 + n_2 - 1)^4 - 2(n_1 + n_2 - 1)^3[M_1(G_1) + M_1(G_2)] \\
&+ n_1n_2^2 + n_2n_1^2 + 4m_1n_2 + 4m_2n_1 + (n_1 + n_2 - 1)^2[F(G_1) + F(G_2)] \\
&+ 3n_2M_1(G_1) + 3n_1M_1(G_2) + 6n_2^2m_1 + 6n_1^2m_2 + n_1n_2^3 + n_2n_1^3 \\
&+ 4(n_1 + n_2 - 1)^2[M_2(G_1) + M_2(G_2) + n_2M_1(G_1) + n_1M_1(G_2)] \\
&+ n_2^2m_1 + n_1^2m_2 + 4m_1m_2 + 2m_1n_1n_2 + 2m_2n_2n_1 + n_1^2n_2^2 \\
&- 2(n_1 + n_2 - 1)(M_1(G_1) + M_1(G_2) + n_1n_2^2 + n_2n_1^2 + 4m_1n_2 \\
&+ 4m_2n_1)[F(G_1) + F(G_2) + 3n_2M_1(G_1) + 3n_1M_1(G_2) \\
&+ 6n_2^2m_1 + 6n_1^2m_2 + n_1n_2^3 + n_2n_1^3] + 2n_2M_1(G_1)F(G_1) \\
&+ 2n_1M_1(G_2)F(G_2) + HM_2(G_1) + HM_2(G_2) + n_2^2F(G_1) + n_1^2F(G_2) \\
&+ 4n_2^2M_2(G_1) + 4n_1^2M_2(G_2) + 2n_2^3M_1(G_1) + 2n_1^3M_1(G_2) + n_1^4m_1 \\
&+ n_1^4m_2 + n_1^3n_2^3 + [4n_1m_2 + n_1^2n_2]M_1(G_1) + [4n_2m_1 + n_1n_2^2]M_1(G_2) \\
&+ 4n_1^2n_2^2[m_1 + m_2] + 16n_1n_2m_1m_2 + M_1(G_1)M_1(G_2).
\end{aligned}$$

**Proof.** By (Theorem 3.1.1) we have

$$\begin{aligned}
HM_2(\overline{G}) &= m(n-1)^4 - 2(n-1)^3M_1(G) + (n-1)^2F(G) + 4(n-1)^2M_2(G) \\
&- 2(n-1)M_1(G)F(G) + HM_2(G).
\end{aligned}$$

60 And  $M_1(G_1 + G_2) = M_1(G_1) + M_1(G_2) + n_1n_2^2 + n_2n_1^2 + 4m_1n_2 + 4m_2n_1$  given in [25].  
 $F(G_1 + G_2) = F(G_1) + F(G_2) + 3n_2M_1(G_1) + 3n_1M_1(G_2) + 6n_2^2m_1 + 6n_1^2m_2 + n_1n_2^3 + n_2n_1^3$   
given in [23].  $|E(G_1 + G_2)| = m_1 + m_2 + n_1n_2$ ,  $|V(G_1 + G_2)| = n_1 + n_2$  and by (Theorem  
3.1.5) and (Theorem 3.1.6). Then,

$$\begin{aligned}
HM_2(\overline{G_1 + G_2}) &= |E(G_1 + G_2)|(|V(G_1 + G_2)| - 1)^4 - 2(|V(G_1 + G_2)| - 1)^3M_1(G_1 + G_2) \\
&+ (|V(G_1 + G_2)| - 1)^2F(G_1 + G_2) + 4(|V(G_1 + G_2)| - 1)^2M_2(G_1 + G_2) \\
&- 2(|V(G_1 + G_2)| - 1)M_1(G_1 + G_2)F(G_1 + G_2) + HM_2(G_1 + G_2) \\
&= (m_1 + m_2 + n_1n_2)(n_1 + n_2 - 1)^4 - 2(n_1 + n_2 - 1)^3[M_1(G_1) + M_1(G_2) \\
&+ n_1n_2^2 + n_2n_1^2 + 4m_1n_2 + 4m_2n_1] + (n_1 + n_2 - 1)^2[F(G_1) + F(G_2) \\
&+ 3n_2M_1(G_1) + 3n_1M_1(G_2) + 6n_2^2m_1 + 6n_1^2m_2 + n_1n_2^3 + n_2n_1^3] \\
&+ 4(n_1 + n_2 - 1)^2[M_2(G_1) + M_2(G_2) + n_2M_1(G_1) + n_1M_1(G_2) \\
&+ n_2^2m_1 + n_1^2m_2 + 4m_1m_2 + 2m_1n_1n_2 + 2m_2n_2n_1 + n_1^2n_2^2] \\
&- 2(n_1 + n_2 - 1)(M_1(G_1) + M_1(G_2) + n_1n_2^2 + n_2n_1^2 + 4m_1n_2 \\
&+ 4m_2n_1)[F(G_1) + F(G_2) + 3n_2M_1(G_1) + 3n_1M_1(G_2) \\
&+ 6n_2^2m_1 + 6n_1^2m_2 + n_1n_2^3 + n_2n_1^3] + 2n_2M_1(G_1)F(G_1) \\
&+ 2n_1M_1(G_2)F(G_2) + HM_2(G_1) + HM_2(G_2) + n_2^2F(G_1) + n_1^2F(G_2) \\
&+ 4n_2^2M_2(G_1) + 4n_1^2M_2(G_2) + 2n_2^3M_1(G_1) + 2n_1^3M_1(G_2) + n_2^4m_1 \\
&+ n_1^4m_2 + n_1^3n_2^3 + [4n_1m_2 + n_1^2n_2]M_1(G_1) + [4n_2m_1 + n_1n_2^2]M_1(G_2) \\
&+ 4n_1^2n_2^2[m_1 + m_2] + 16n_1n_2m_1m_2 + M_1(G_1)M_1(G_2).
\end{aligned}$$

**Definition 3.1.8** [20, 21] *The strong product  $G_1 * G_2$  of two graphs  $G_1$  and  $G_2$  is a*  
65 *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  $\{ u_1 = u_2 \in V(G_1) \text{ and } v_1v_2 \in E(G_2) \}$  or  $\{ v_1 = v_2 \in V(G_2)$*   
*and  $u_1u_2 \in E(G_1) \}$ , such that  $|V(G_1 * G_2)| = n_1n_2$ ,  $|E(G_1 * G_2)| = m_1n_2 + n_1m_2 + 2m_1m_2$*   
*and  $\delta_{G_1 * G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v) + \delta_{G_1}(u)\delta_{G_2}(v)$ .*

**Theorem 3.1.9** [15] The first and second Hyper-Zagreb index are given by:

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

$$\begin{aligned}
M_2(G_1 * G_2) &= (n_2 + 5m_2)M_2(G_1) + (n_1 + 5m_1)M_2(G_2) + 3m_2M_1(G_1) + 3m_1M_1(G_2) \\
&+ 3M_1(G_1)M_1(G_2) + 2M_1(G_2)M_2(G_1) + 2M_1(G_1)M_2(G_2) + M_2(G_1)M_2(G_2).
\end{aligned}$$

**Theorem 3.1.10** The second Hyper-Zagreb index of complement  $G_1 * G_2$  is given by:

$$\begin{aligned}
HM_2(\overline{G_1 * G_2}) &= [m_1n_2 + n_1m_2 + 2m_1m_2](n_1n_2 - 1)^4 \\
&- 2(n_1n_2 - 1)^3[(n_2 + 6m_2)M_1(G_1) + 8m_2m_1 + (6m_1 + n_1)M_1(G_2) \\
&+ 2M_1(G_1)M_1(G_2)] + (n_1n_2 - 1)^2[n_2F(G_1) + n_1F(G_2) \\
&+ F(G_1)F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2) + 6m_2F(G_1) \\
&+ 6m_1F(G_2) + 3F(G_2)M_1(G_1) + 3F(G_1)M_1(G_2) + 6M_1(G_1)M_1(G_2)] \\
&+ 4(n_1n_2 - 1)^2[(n_2 + 5m_2)M_2(G_1) + (n_1 + 5m_1)M_2(G_2) + 3m_2M_1(G_1) \\
&+ 3m_1M_1(G_2) + 3M_1(G_1)M_1(G_2) + 2M_1(G_2)M_2(G_1) + 2M_1(G_1)M_2(G_2) \\
&+ M_2(G_1)M_2(G_2)] - 2(n_1n_2 - 1)[(n_2 + 6m_2)M_1(G_1) + 8m_2m_1 \\
&+ (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)][n_2F(G_1) + n_1F(G_2) \\
&+ F(G_1)F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2) + 6m_2F(G_1) + 6m_1F(G_2) \\
&+ 3F(G_2)M_1(G_1) + 3F(G_1)M_1(G_2) + 6M_1(G_1)M_1(G_2)] \\
&+ HM_2(G_2)[n_1 + 10m_1 + 10M_1(G_1) + 8M_2(G_1) \\
&+ 6F(G_1) + 4ReZG_3(G_1) + Y(G_1)] + HM_2(G_1)[n_2 + 10m_2 \\
&+ 10M_1(G_2) + 8M_2(G_2) + 6F(G_2) + 4ReZG_3(G_2) + Y(G_2)] \\
&+ Y(G_2)[m_1 + 2M_1(G_1) + 4M_2(G_1) + F(G_1) + 2ReZG_3(G_1)] \\
&+ Y(G_1)[m_2 + 2M_1(G_2) + 4M_2(G_2) + F(G_2) + 2ReZG_3(G_2)] \\
&+ 4ReZG_3(G_2)[m_1 + 2M_1(G_1) + 2M_2(G_1) + 2F(G_1)] \\
&+ 4ReZG_3(G_1)[m_2 + 2M_1(G_2) + 2M_2(G_2) + 2F(G_2)] \\
&+ F(G_2)[3M_1(G_1) + 8M_2(G_1)] + F(G_1)[3M_1(G_2) + 8M_2(G_2)] \\
&+ 8M_2(G_1)M_2(G_2) + 4M_1(G_1)M_2(G_2) + 4M_1(G_2)M_2(G_1) \\
&+ 2HM_2(G_1)HM_2(G_2) + 5F(G_1)F(G_2) + 6ReZG_3(G_1)ReZG_3(G_2).
\end{aligned}$$

**Proof.** By using (Theorem 3.1.1) we have,

$$\begin{aligned}
HM_2(\overline{G_1 * G_2}) &= |E(G_1 * G_2)|(|V(G_1 * G_2)| - 1)^4 - 2(|V(G_1 * G_2)| - 1)^3M_1(G_1 * G_2) \\
&+ (|V(G_1 * G_2)| - 1)^2F(G_1 * G_2) + 4(|V(G_1 * G_2)| - 1)^2M_2(G_1 * G_2) \\
&- 2(|V(G_1 * G_2)| - 1)M_1(G_1 * G_2)F(G_1 * G_2) + HM_2(G_1 * G_2),
\end{aligned}$$

And by [23, 12], respectively, we have

$$\begin{aligned}
F(G_1 * G_2) &= n_2F(G_1) + n_1F(G_2) + F(G_1)F(G_2) + 6m_2M_1(G_1) \\
&+ 6m_1M_1(G_2) + 6m_2F(G_1) + 6m_1F(G_2) + 3F(G_2)M_1(G_1) \\
&+ 3F(G_1)M_1(G_2) + 6M_1(G_1)M_1(G_2).
\end{aligned}$$

$$\begin{aligned}
HM_2(G_1 * G_2) &= HM_2(G_2)[n_1 + 10m_1 + 10M_1(G_1) + 8M_2(G_1) \\
&+ 6F(G_1) + 4ReZG_3(G_1) + Y(G_1)] + HM_2(G_1)[n_2 + 10m_2 \\
&+ 10M_1(G_2) + 8M_2(G_2) + 6F(G_2) + 4ReZG_3(G_2) + Y(G_2)] \\
&+ Y(G_2)[m_1 + 2M_1(G_1) + 4M_2(G_1) + F(G_1) + 2ReZG_3(G_1)] \\
&+ Y(G_1)[m_2 + 2M_1(G_2) + 4M_2(G_2) + F(G_2) + 2ReZG_3(G_2)] \\
&+ 4ReZG_3(G_2)[m_1 + 2M_1(G_1) + 2M_2(G_1) + 2F(G_1)] \\
&+ 4ReZG_3(G_1)[m_2 + 2M_1(G_2) + 2M_2(G_2) + 2F(G_2)] \\
&+ F(G_2)[3M_1(G_1) + 8M_2(G_1)] + F(G_1)[3M_1(G_2) + 8M_2(G_2)] \\
&+ 8M_2(G_1)M_2(G_2) + 4M_1(G_1)M_2(G_2) + 4M_1(G_2)M_2(G_1) \\
&+ 2HM_2(G_1)HM_2(G_2) + 5F(G_1)F(G_2) + 6ReZG_3(G_1)ReZG_3(G_2).
\end{aligned}$$

And since  $|E(G_1 * G_2)| = m_1n_2 + n_1m_2 + 2m_1m_2$ ,  $|V(G_1 * G_2)| = n_1n_2$  and by (Theorem 3.1.9). Which are complete the proof.

**Definition 3.1.11** [20, 21] *The Cartesian product  $G_1 \times G_2$  of two 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  $x = y$ , such that  $|V(G_1 \times G_2)| = n_1n_2$ ,  $|E(G_1 \times G_2)| = m_1n_2 + n_1m_2$ , and  $\delta_{G_1 \times G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v)$ .*

**Theorem 3.1.12** The second Hyper-Zagreb index of complement  $G_1 \times G_2$  is given by:

$$\begin{aligned} HM_2(\overline{G_1 \times G_2}) &= (m_1n_2 + n_1m_2)(n_1n_2 - 1)^4 - 2(n_1n_2 - 1)^3[n_2M_1(G_1) + n_1M_1(G_2) \\ &+ 8m_1m_2] + (n_1n_2 - 1)^2[n_2F(G_1) + n_1F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2)] \\ &+ 4(n_1n_2 - 1)^2[3m_2M_1(G_1) + 3m_1M_1(G_2) + n_1M_2(G_2) + n_2M_2(G_1)] \\ &- 2(n_1n_2 - 1)[n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2][n_2F(G_1) + n_1F(G_2) \\ &+ 6m_2M_1(G_1) + 6m_1M_1(G_2)] + n_2HM_2(G_1) + n_1HM_2(G_2) \\ &+ 3F(G_1)M_1(G_2) + 3F(G_2)M_1(G_1) + m_1[Y(G_2) + 4ReZG_3(G_2)] \\ &+ m_2[Y(G_1) + 4ReZG_3(G_1)] + 4M_1(G_1)M_2(G_2) + 4M_1(G_2)M_2(G_1). \end{aligned}$$

**Proof.** By (Theorem 3.1.1) we have

$$\begin{aligned} HM_2(\overline{G}) &= |E(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1)^4 - 2(|V(G_1 \times G_2)| - 1)^3M_1(G_1 \times G_2) \\ &+ (|V(G_1 \times G_2)| - 1)^2F(G_1 \times G_2) + 4(|V(G_1 \times G_2)| - 1)^2M_2(G_1 \times G_2) \\ &- 2(|V(G_1 \times G_2)| - 1)M_1(G_1 \times G_2)F(G_1 \times G_2) + HM_2(G_1 \times G_2). \end{aligned}$$

And  $M_1(G_1 \times G_2) = n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2$ ,  $M_2(G_1 \times G_2) = 3m_2M_1(G_1) + 3m_1M_1(G_2) + n_1M_2(G_2) + n_2M_2(G_1)$  given in [20].  $F(G_1 \times G_2) = n_2F(G_1) + n_1F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2)$  given in [23].  $HM_2(G_1 \times G_2) = n_2HM_2(G_1) + n_1HM_2(G_2) + 3F(G_1)M_1(G_2) + 3F(G_2)M_1(G_1) + m_1[Y(G_2) + 4ReZG_3(G_2)] + m_2[Y(G_1) + 4ReZG_3(G_1)] + 4M_1(G_1)M_2(G_2) + 4M_1(G_2)M_2(G_1)$  given in [12] and since  $|E(G_1 \times G_2)| = m_1n_2 + n_1m_2$ ,  $|V(G_1 \times G_2)| = n_1n_2$ . Which are complete the proof.

**Definition 3.1.13** [20, 21] *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  $v_2\}$ , such that  $|V(G_1 \circ G_2)| = n_1n_2$ ,  $|E(G_1 \circ G_2)| = m_1n_2^2 + m_2n_1$  and  $\delta_{G_1 \circ G_2}(u, v) = n_2\delta_{G_1}(u) + \delta_{G_2}(v)$ .*

**Theorem 3.1.14** The second Hyper-Zagreb index of complement  $G_1 \circ G_2$  is given by:

$$\begin{aligned} HM_2(\overline{G_1 \circ G_2}) &= (m_1n_2^2 + m_2n_1)(n_1n_2 - 1)^4 - 2(n_1n_2 - 1)^3[n_2^3M_1(G_1) \\ &+ n_1M_1(G_2) + 8n_2m_2m_1] + (n_1n_2 - 1)^2[n_2^4F(G_1) + n_1F(G_2) \\ &+ 6n_2^2m_2M_1(G_1) + 6n_2m_1M_1(G_2)] + 4(n_1n_2 - 1)^2[n_2^4M_2(G_1) \\ &+ n_1M_2(G_2) + 3n_2^2m_2M_1(G_1) + 2n_2m_1M_1(G_2) + 4m_1m_2^2] \\ &- 2(n_1n_2 - 1)[n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1][n_2^4F(G_1) \\ &+ n_1F(G_2) + 6n_2^2m_2M_1(G_1) + 6n_2m_1M_1(G_2)] \\ &+ n_2^6HM_2(G_1) + n_1HM_2(G_2) + n_2^4m_2[Y(G_1) + 4ReZG_3(G_1)] \\ &+ 4n_2m_1ReZG_3(G_2) + 3n_2^2F(G_1)M_1(G_2) + n_2^2M_1(G_1)[F(G_2) \\ &+ 4M_2(G_2)] + m_1M_1^2(G_2) + 4n_2m_2[4n_2m_2M_2(G_1) + M_1(G_1)M_1(G_2)]. \end{aligned}$$

95 **Proof.** By using (Theorem 3.1.1) we have,

$$\begin{aligned} HM_2(\overline{G_1 \circ G_2}) &= |E(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1)^4 - 2(|V(G_1 \circ G_2)| - 1)^3 M_1(G_1 \circ G_2) \\ &+ (|V(G_1 \circ G_2)| - 1)^2 F(G_1 \circ G_2) + 4(|V(G_1 \circ G_2)| - 1)^2 M_2(G_1 \circ G_2) \\ &- 2(|V(G_1 \circ G_2)| - 1) M_1(G_1 \circ G_2) F(G_1 \circ G_2) + HM_2(G_1 \circ G_2), \end{aligned}$$

And by [20], [23], and [12], respectively, we have

$$M_1(G_1 \circ G_2) = n_2^3 M_1(G_1) + n_1 M_1(G_2) + 8n_2 m_2 m_1,$$

$$\begin{aligned} M_2(G_1 \circ G_2) &= n_2^4 M_2(G_1) + n_1 M_2(G_2) + 3n_2^2 m_2 M_1(G_1) \\ &+ 2n_2 m_1 M_1(G_2) + 4m_1 m_2^2, \end{aligned}$$

$$F(G_1 \circ G_2) = n_2^4 F(G_1) + n_1 F(G_2) + 6n_2^2 m_2 M_1(G_1) + 6n_2 m_1 M_1(G_2),$$

$$\begin{aligned} HM_2(G_1 \circ G_2) &= n_2^6 HM_2(G_1) + n_1 HM_2(G_2) + n_2^4 m_2 [Y(G_1) + 4ReZG_3(G_1)] \\ &+ 4n_2 m_1 ReZG_3(G_2) + 3n_2^2 F(G_1) M_1(G_2) + n_2^2 M_1(G_1) [F(G_2) \\ &+ 4M_2(G_2)] + m_1 M_1^2(G_2) + 4n_2 m_2 [4n_2 m_2 M_2(G_1) + M_1(G_1) M_1(G_2)], \end{aligned}$$

And since  $|E(G_1 \circ G_2)| = m_1 n_2^2 + m_2 n_1$ ,  $|V(G_1 \circ G_2)| = n_1 n_2$ .

100 Which are complete the proof.

**Definition 3.1.15** [20, 21] *The disjunction  $G_1 \vee G_2$  of two 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  $(v_1, v_2) \in E(G_2)$ , such that  $|V(G_1 \vee G_2)| = n_1 n_2$ ,  $|E(G_1 \vee G_2)| = m_1 n_2^2 + m_2 n_1^2 - 2m_1 m_2$  and  $\delta_{G_1 \vee G_2}(u, v) = n_2 \delta_{G_1}(u) + n_1 \delta_{G_2}(v) - \delta_{G_1}(u) \delta_{G_2}(v)$ .*

**Theorem 3.1.16** The second Hyper-Zagreb index of complement  $G_1 \vee G_2$  is given by:

$$\begin{aligned}
HM_2(\overline{G_1 \vee G_2}) &= [m_1 n_2^2 + m_2 n_1^2 - 2m_1 m_2](n_1 n_2 - 1)^4 - 2(n_1 n_2 - 1)^3 [(n_1 n_2^2 \\
&\quad - 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) \\
&\quad + 8m_1 m_2 n_1 n_2] + (n_1 n_2 - 1)^2 [n_2^4 F(G_1) + n_1^4 F(G_2) - F(G_1)F(G_2) \\
&\quad + 6n_1 n_2^2 m_2 M_1(G_1) + 6n_2 n_1^2 m_1 M_1(G_2) + 3n_2 F(G_1)M_1(G_2) \\
&\quad + 3n_1 F(G_2)M_1(G_1) - 6n_2^2 m_2 F(G_1) - 6n_1^2 m_1 F(G_2) - 6n_1 n_2 M_1(G_1)M_1(G_2)] \\
&+ 4(n_1 n_2 - 1)^2 [(n_1^2 - 2m_1)^2 - 2n_1^2 m_1]M_2(G_2) + ((n_2^2 - 2m_2)^2 \\
&\quad - 2n_2^2 m_2)M_2(G_1) + (2n_1^2 n_2 m_1 - 4m_1^2 n_2)M_1(G_2) \\
&\quad + (2n_2^2 n_1 m_2 - 4m_2^2 n_1)M_1(G_1) - n_1 n_2 M_1(G_2)M_1(G_1) \\
&\quad + 2n_2 M_2(G_1)M_1(G_2) + 2n_1 M_2(G_2)M_1(G_1) - 2M_2(G_2)M_2(G_1) \\
&\quad + 4m_2 m_1 (n_2^2 m_1 + n_1^2 m_2)] - 2(n_1 n_2 - 1) [(n_1 n_2^2 \\
&\quad - 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) \\
&\quad + 8m_1 m_2 n_1 n_2] [n_2^4 F(G_1) + n_1^4 F(G_2) - F(G_1)F(G_2) \\
&\quad + 6n_1 n_2^2 m_2 M_1(G_1) + 6n_2 n_1^2 m_1 M_1(G_2) + 3n_2 F(G_1)M_1(G_2) \\
&\quad + 3n_1 F(G_2)M_1(G_1) - 6n_2^2 m_2 F(G_1) - 6n_1^2 m_1 F(G_2) - 6n_1 n_2 M_1(G_1)M_1(G_2)] \\
&+ [HM_2(G_2)[n_1(n_1^5 + 16n_1 m_1^2 - 10n_1^3 m_1 - 8n_1 M_2(G_1)) \\
&\quad - 2n_1 F(G_1) + 4ReZG_3(G_1)) + M_1(G_1)(M_1(G_1) + 6n_1^3 - 8n_1 m_1)] \\
&\quad + n_2^2 F(G_2)M_1(G_1)[n_1^3 - 4n_1 m_1 + M_1(G_1)] + HM_2(G_1)[n_2(n_2^5 \\
&\quad + 16n_2 m_2^2 - 10n_2^3 m_2 - 8n_2 M_2(G_2) - 2n_2 F(G_2) + 4ReZG_3(G_2)) \\
&\quad + M_1(G_2)(M_1(G_2) + 6n_2^3 - 8n_2 m_2)] + n_1^2 F(G_1)M_1(G_2)[n_2^3 \\
&\quad - 4n_2 m_2 + M_1(G_2)] + 2n_2 ReZG_3(G_2)[n_1^2(2n_1^2 m_1 + F(G_1) - 8m_1^2 \\
&\quad + 4M_2(G_1)) - M_1(G_1)(M_1(G_1) + 2n_1^3 - 6n_1 m_1)] + 4n_2^2 M_2(G_2)[4n_1^2 m_1^2 \\
&\quad + M_1^2(G_1) - 4n_1 m_1 M_1(G_1)] + 2n_1 ReZG_3(G_1)[n_2^2(2n_2^2 m_2 + F(G_2) \\
&\quad - 8m_2^2 + 4M_2(G_2)) - M_1(G_2)(M_1(G_2) + 2n_2^3 - 6n_2 m_2)] \\
&\quad + 4n_1^2 M_2(G_1)[4n_2^2 m_2^2 + M_1^2(G_2) - 4n_2 m_2 M_1(G_2)] \\
&\quad + 2M_1(G_1)M_1(G_2)[n_1^3(2n_2 m_2 - M_1(G_2)) + n_2^3(2n_1 m_1 - M_1(G_1))] \\
&\quad + n_1^4 m_1 M_1^2(G_2) + n_2^4 m_2 M_1^2(G_1) - 6n_1 n_2 ReZG_3(G_1)ReZG_3(G_2) \\
&\quad - n_1^2 n_2^2 [F(G_1)F(G_2) + 8M_2(G_1)M_2(G_2)] - 2HM_2(G_1)HM_2(G_2)]
\end{aligned}$$

**Proof.** By using (Theorem 3.1.1) we have,

$$\begin{aligned}
HM_2(\overline{G_1 \vee G_2}) &= |E(G_1 \vee G_2)|(|V(G_1 \vee G_2)| - 1)^4 - 2(|V(G_1 \vee G_2)| - 1)^3 M_1(G_1 \vee G_2) \\
&\quad + (|V(G_1 \vee G_2)| - 1)^2 F(G_1 \vee G_2) + 4(|V(G_1 \vee G_2)| - 1)^2 M_2(G_1 \vee G_2) \\
&\quad - 2(|V(G_1 \vee G_2)| - 1)M_1(G_1 \vee G_2)F(G_1 \vee G_2) + HM_2(G_1 \vee G_2),
\end{aligned}$$

And by [25, 27], [23], [24] and [12], respectively, we have

$$\begin{aligned}
M_1(G_1 \vee G_2) &= (n_1 n_2^2 - 4m_2 n_2)M_1(G_1) + M_1(G_2)M_1(G_1) \\
&\quad + (n_2 n_1^2 - 4m_1 n_1)M_1(G_2) + 8m_1 m_2 n_1 n_2.
\end{aligned}$$

$$\begin{aligned}
M_2(G_1 \vee G_2) &= ((n_1^2 - 2m_1)^2 - 2n_1^2 m_1)M_2(G_2) + ((n_2^2 - 2m_2)^2 \\
&\quad - 2n_2^2 m_2)M_2(G_1) + (2n_1^2 n_2 m_1 - 4m_1^2 n_2)M_1(G_2) \\
&\quad + (2n_2^2 n_1 m_2 - 4m_2^2 n_1)M_1(G_1) - n_1 n_2 M_1(G_2)M_1(G_1) \\
&\quad + 2n_2 M_2(G_1)M_1(G_2) + 2n_1 M_2(G_2)M_1(G_1) - 2M_2(G_2)M_2(G_1) \\
&\quad + 4m_2 m_1 (n_2^2 m_1 + n_1^2 m_2).
\end{aligned}$$

$$\begin{aligned}
F(G_1 \vee G_2) &= n_2^4 F(G_1) + n_1^4 F(G_2) - F(G_1)F(G_2) + 6n_1 n_2^2 m_2 M_1(G_1) \\
&\quad + 6n_2 n_1^2 m_1 M_1(G_2) + 3n_2 F(G_1)M_1(G_2) + 3n_1 F(G_2)M_1(G_1) \\
&\quad - 6n_2^2 m_2 F(G_1) - 6n_1^2 m_1 F(G_2) - 6n_1 n_2 M_1(G_1)M_1(G_2).
\end{aligned}$$

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$$\begin{aligned}
HM_2(G_1 \vee G_2) &= HM_2(G_2)[n_1(n_1^5 + 16n_1 m_1^2 - 10n_1^3 m_1 - 8n_1 M_2(G_1) \\
&\quad - 2n_1 F(G_1) + 4ReZG_3(G_1)) + M_1(G_1)(M_1(G_1) + 6n_1^3 - 8n_1 m_1)] \\
&\quad + n_2^2 F(G_2)M_1(G_1)[n_1^3 - 4n_1 m_1 + M_1(G_1)] + HM_2(G_1)[n_2(n_2^5 \\
&\quad + 16n_2 m_2^2 - 10n_2^3 m_2 - 8n_2 M_2(G_2) - 2n_2 F(G_2) + 4ReZG_3(G_2)) \\
&\quad + M_1(G_2)(M_1(G_2) + 6n_2^3 - 8n_2 m_2)] + n_1^2 F(G_1)M_1(G_2)[n_2^3 \\
&\quad - 4n_2 m_2 + M_1(G_2)] + 2n_2 ReZG_3(G_2)[n_1^2(2n_1^2 m_1 + F(G_1) - 8m_1^2 \\
&\quad + 4M_2(G_1)) - M_1(G_1)(M_1(G_1) + 2n_1^3 - 6n_1 m_1)] + 4n_2^2 M_2(G_2)[4n_1^2 m_1^2 \\
&\quad + M_1^2(G_1) - 4n_1 m_1 M_1(G_1)] + 2n_1 ReZG_3(G_1)[n_2^2(2n_2^2 m_2 + F(G_2) \\
&\quad - 8m_2^2 + 4M_2(G_2)) - M_1(G_2)(M_1(G_2) + 2n_2^3 - 6n_2 m_2)] \\
&\quad + 4n_1^2 M_2(G_1)[4n_2^2 m_2^2 + M_1^2(G_2) - 4n_2 m_2 M_1(G_2)] \\
&\quad + 2M_1(G_1)M_1(G_2)[n_1^3(2n_2 m_2 - M_1(G_2)) + n_2^3(2n_1 m_1 - M_1(G_1))] \\
&\quad + n_1^4 m_1 M_1^2(G_2) + n_2^4 m_2 M_1^2(G_1) - 6n_1 n_2 ReZG_3(G_1)ReZG_3(G_2) \\
&\quad - n_1^2 n_2^2 [F(G_1)F(G_2) + 8M_2(G_1)M_2(G_2)] - 2HM_2(G_1)HM_2(G_2),
\end{aligned}$$

And since  $|E(G_1 \vee G_2)| = m_1 n_2^2 + m_2 n_1^2 - 2m_1 m_2$ ,  $|V(G_1 \vee G_2)| = n_1 n_2$ .  
Which are complete the proof.

**Definition 3.1.17** [20, 21] *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  $E(G_1 \oplus G_2) = (u_1, u_2)(v_1, v_2) | u_1 v_1 \in E(G_1)$  or  $u_2 v_2 \in E(G_2)$  but not both, such that  $|V(G_1 \oplus G_2)| = n_1 n_2$ ,  $|E(G_1 \oplus G_2)| = m_1 n_2^2 + m_2 n_1^2 - 4m_1 m_2$  and  $\delta_{G_1 \oplus G_2}(u, v) = n_2 \delta_{G_1}(u) + n_1 \delta_{G_2}(v) - 2\delta_{G_1}(u)\delta_{G_2}(v)$ .*

**Theorem 3.1.18** The second Hyper-Zagreb index of complement  $G_1 \oplus G_2$  is given

by:

$$\begin{aligned}
HM_2(\overline{G_1 \oplus G_2}) &= [m_1 n_2^2 + m_2 n_1^2 - 4m_1 m_2](n_1 n_2 - 1)^4 - 2(n_1 n_2 - 1)^3 [(n_1 n_2^2 \\
&\quad - 8m_2 n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2 n_1^2 - 8m_1 n_1)M_1(G_2) \\
&\quad + 8m_1 m_2 n_1 n_2] + (n_1 n_2 - 1)^2 [n_2^4 F(G_1) + n_1^4 F(G_2) - 8F(G_1)F(G_2) \\
&\quad + 6n_1 n_2^2 m_2 M_1(G_1) + 6n_2 n_1^2 m_1 M_1(G_2) + 12n_2 F(G_1)M_1(G_2) \\
&\quad + 12n_1 F(G_2)M_1(G_1) - 12n_2^2 m_2 F(G_1) - 12n_1^2 m_1 F(G_2) \\
&\quad - 12n_1 n_2 M_1(G_1)M_1(G_2)] + 4(n_1 n_2 - 1)^2 [((n_1^2 - 2m_1)^2 - 4n_1^2 m_1)M_2(G_2) \\
&\quad + ((n_2^2 - 2m_2)^2 - 4n_2^2 m_2)M_2(G_1) + (2n_1^2 n_2 m_1 - 8m_1^2 n_2)M_1(G_2) \\
&\quad + (2n_2^2 n_1 m_2 - 8m_2^2 n_1)M_1(G_1) - 2n_1 n_2 M_1(G_2)M_1(G_1) \\
&\quad + 8n_2 M_2(G_1)M_1(G_2) + 8n_1 M_2(G_2)M_1(G_1) - 16M_2(G_2)M_2(G_1) \\
&\quad + 4m_2 m_1 (n_2^2 m_1 + n_1^2 m_2)] - 2(n_1 n_2 - 1) [(n_1 n_2^2 \\
&\quad - 8m_2 n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2 n_1^2 - 8m_1 n_1)M_1(G_2) \\
&\quad + 8m_1 m_2 n_1 n_2] [n_2^4 F(G_1) + n_1^4 F(G_2) - 8F(G_1)F(G_2) \\
&\quad + 6n_1 n_2^2 m_2 M_1(G_1) + 6n_2 n_1^2 m_1 M_1(G_2) + 12n_2 F(G_1)M_1(G_2) \\
&\quad + 12n_1 F(G_2)M_1(G_1) - 12n_2^2 m_2 F(G_1) - 12n_1^2 m_1 F(G_2) \\
&\quad - 12n_1 n_2 M_1(G_1)M_1(G_2)] + [HM_2(G_2)[n_1(n_1^5 + 64n_1 m_1^2 - 20n_1^3 m_1 \\
&\quad - 64n_1 M_2(G_1) - 16n_1 F(G_1) + 64ReZG_3(G_1)) + M_1(G_1)(16M_1(G_1) \\
&\quad + 24n_1^3 - 64n_1 m_1)] + n_2^2 F(G_2)M_1(G_1)[n_1^3 - 8n_1 m_1 + 4M_1(G_1)] \\
&\quad + HM_2(G_1)[n_2(n_2^5 + 64n_2 m_2^2 - 20n_2^3 m_2 - 64n_2 M_2(G_2) - 16n_2 F(G_2) \\
&\quad + 64ReZG_3(G_2)) + M_1(G_2)(16M_1(G_2) + 24n_2^3 - 64n_2 m_2)] \\
&\quad + n_1^2 F(G_1)M_1(G_2)[n_2^3 - 8n_2 m_2 + 4M_1(G_2)] + 4n_2 ReZG_3(G_2) \\
&\quad \cdot [n_1^2(2n_1^2 m_1 + 2F(G_1) - 8m_1^2 + 8M_2(G_1)) - M_1(G_1)(4M_1(G_1) \\
&\quad + 2n_1^3 - 12n_1 m_1)] + 16n_2^2 M_2(G_2)[n_1^2 m_1^2 + M_1^2(G_1) - 2n_1 m_1 M_1(G_1)] \\
&\quad + 4n_1 ReZG_3(G_1)[n_2^2(n_2^2 m_2 + 2F(G_2) - 8m_2^2 + 8M_2(G_2)) \\
&\quad - M_1(G_2)(4M_1(G_2) + 2n_2^3 - 12n_2 m_2)] + 16n_1^2 M_2(G_1)[n_2^2 m_2^2 \\
&\quad + M_1^2(G_2) - 2n_2 m_2 M_1(G_2)] + 4M_1(G_1)M_1(G_2)[n_1^3[n_2 m_2 - M_1(G_2)] \\
&\quad + n_2^3(n_1 m_1 - M_1(G_1))] + n_1^4 m_1 M_1^2(G_2) + n_2^4 m_2 M_1^2(G_1) \\
&\quad - 48n_1 n_2 ReZG_3(G_1)ReZG_3(G_2) - 2n_1^2 n_2^2 [F(G_1)F(G_2) \\
&\quad + 8M_2(G_1)M_2(G_2)] - 64HM_2(G_1)HM_2(G_2)].
\end{aligned}$$

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**Proof.** By using (Theorem 3.1.1) we have,

$$\begin{aligned}
HM_2(\overline{G_1 \oplus G_2}) &= |E(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)^4 - 2(|V(G_1 \oplus G_2)| - 1)^3 M_1(G_1 \oplus G_2) \\
&\quad + (|V(G_1 \oplus G_2)| - 1)^2 F(G_1 \oplus G_2) + 4(|V(G_1 \oplus G_2)| - 1)^2 M_2(G_1 \oplus G_2) \\
&\quad - 2(|V(G_1 \oplus G_2)| - 1)M_1(G_1 \oplus G_2)F(G_1 \oplus G_2) + HM_2(G_1 \oplus G_2),
\end{aligned}$$

And by [25, 27], [23], [24] and [12], respectively, we have

$$\begin{aligned}
M_1(G_1 \oplus G_2) &= (n_1 n_2^2 - 8m_2 n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) \\
&\quad + (n_2 n_1^2 - 8m_1 n_1)M_1(G_2) + 8m_1 m_2 n_1 n_2.
\end{aligned}$$

$$\begin{aligned}
M_2(G_1 \oplus G_2) &= ((n_1^2 - 2m_1)^2 - 4n_1^2 m_1)M_2(G_2) + ((n_2^2 - 2m_2)^2 \\
&- 4n_2^2 m_2)M_2(G_1) + (2n_1^2 n_2 m_1 - 8m_1^2 n_2)M_1(G_2) \\
&+ (2n_2^2 n_1 m_2 - 8m_2^2 n_1)M_1(G_1) - 2n_1 n_2 M_1(G_2)M_1(G_1) \\
&+ 8n_2 M_2(G_1)M_1(G_2) + 8n_1 M_2(G_2)M_1(G_1) - 16M_2(G_2)M_2(G_1) \\
&+ 4m_2 m_1 (n_2^2 m_1 + n_1^2 m_2).
\end{aligned}$$

$$\begin{aligned}
F(G_1 \oplus G_2) &= n_2^4 F(G_1) + n_1^4 F(G_2) - 8F(G_1)F(G_2) + 6n_1 n_2^2 m_2 M_1(G_1) \\
&+ 6n_2 n_1^2 m_1 M_1(G_2) + 12n_2 F(G_1)M_1(G_2) + 12n_1 F(G_2)M_1(G_1) \\
&- 12n_2^2 m_2 F(G_1) - 12n_1^2 m_1 F(G_2) - 12n_1 n_2 M_1(G_1)M_1(G_2).
\end{aligned}$$

$$\begin{aligned}
HM_2(G_1 \oplus G_2) &= HM_2(G_2)[n_1(n_1^5 + 64n_1 m_1^2 - 20n_1^3 m_1 - 64n_1 M_2(G_1)) \\
&- 16n_1 F(G_1) + 64ReZG_3(G_1)] + M_1(G_1)(16M_1(G_1) \\
&+ 24n_1^3 - 64n_1 m_1) + n_2^2 F(G_2)M_1(G_1)[n_1^3 - 8n_1 m_1 + 4M_1(G_1)] \\
&+ HM_2(G_1)[n_2(n_2^5 + 64n_2 m_2^2 - 20n_2^3 m_2 - 64n_2 M_2(G_2) - 16n_2 F(G_2) \\
&+ 64ReZG_3(G_2)) + M_1(G_2)(16M_1(G_2) + 24n_2^3 - 64n_2 m_2)] \\
&+ n_1^2 F(G_1)M_1(G_2)[n_2^3 - 8n_2 m_2 + 4M_1(G_2)] + 4n_2 ReZG_3(G_2) \\
&\cdot [n_1^2(2n_1^2 m_1 + 2F(G_1) - 8m_1^2 + 8M_2(G_1)) - M_1(G_1)(4M_1(G_1) \\
&+ 2n_1^3 - 12n_1 m_1)] + 16n_2^2 M_2(G_2)[n_1^2 m_1^2 + M_1^2(G_1) - 2n_1 m_1 M_1(G_1)] \\
&+ 4n_1 ReZG_3(G_1)[n_2^2(n_2^2 m_2 + 2F(G_2) - 8m_2^2 + 8M_2(G_2)) \\
&- M_1(G_2)(4M_1(G_2) + 2n_2^3 - 12n_2 m_2)] + 16n_1^2 M_2(G_1)[n_2^2 m_2^2 \\
&+ M_1^2(G_2) - 2n_2 m_2 M_1(G_2)] + 4M_1(G_1)M_1(G_2)[n_1^3[n_2 m_2 - M_1(G_2)] \\
&+ n_2^3(n_1 m_1 - M_1(G_1))] + n_1^4 m_1 M_1^2(G_2) + n_2^4 m_2 M_1^2(G_1) \\
&- 48n_1 n_2 ReZG_3(G_1)ReZG_3(G_2) - 2n_1^2 n_2^2 [F(G_1)F(G_2) \\
&+ 8M_2(G_1)M_2(G_2)] - 64HM_2(G_1)HM_2(G_2),
\end{aligned}$$

125 And since  $|E(G_1 \oplus G_2)| = m_1 n_2^2 + m_2 n_1^2 - 4m_1 m_2$ ,  $|V(G_1 \oplus G_2)| = n_1 n_2$ .  
Which are complete the proof.

### 3.2. Second Hyper-Zagreb index of complement V-Phenylenic Nanotubes $VPHX[q, p]$ ( $\forall p, q \in \mathbb{N} - \{1\}$ )

130 **Corollary 3.2.1** The second Hyper-Zagreb index of complement  $VPHX[q, p]$  nanotube (Fig 1,2.) is given by

$$\begin{aligned}
HM_2(\overline{VPHX[q, p]}) &= (9pq - q)(6pq - 1)^4 - 2(6pq - 1)^3[54pq - 10q] \\
&+ (6pq - 1)^2[162pq - 38q] + 4(6pq - 1)[81pq + 3q] \\
&- 8q(6pq - 1)[54pq - 10q](162pq - 38q) + 9q(81p - 29).
\end{aligned}$$

Table 1: The edge and vertex partitions of  $VPHX[q, p]$  nanotubes.

Edge partition	$E_5 = E_6^*$	$E_6 = E_9^*$	Vertex partition	$V_2$	$V_3$
Cardinality	$4q$	$9pq - 5q$	Cardinality	$q + q$	$6pq - 2q$

The edge set of  $VPHX[q, p]$  is divided into two edge partitions based on the sum of degrees of the end vertices as:

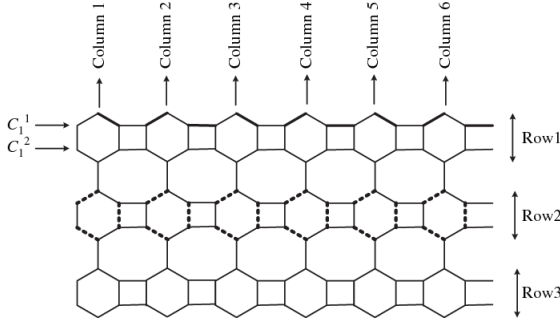


Figure 1:  $VPHX[3,6]$  nanotube

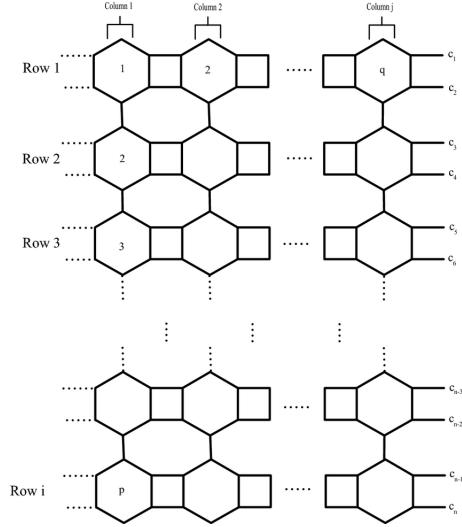


Figure 2: The molecular graph of  $VPHX[q,p]$  nanotube.

$$E_5(VPHX[q,p]) = E_6^* = \{e = uv \in E(VPHX[q,p]) : \delta(u) = 2, \delta(v) = 3\},$$

$$E_6(VPHX[q,p]) = E_9^* = \{e = uv \in E(VPHX[q,p]) : \delta(u) = 3, \delta(v) = 3\},$$

135 **Proof.** By using (Theorem 3.1.1) we have

$$\begin{aligned} HM_2(\overline{VPHX[q,p]}) &= |E(VPHX[q,p])|(|V(VPHX[q,p])| - 1)^4 \\ &\quad - 2(|V(VPHX[q,p])| - 1)^3 M_1(VPHX[q,p]) \\ &\quad + (|V(VPHX[q,p])| - 1)^2 F(VPHX[q,p]) \\ &\quad + 4(|V(VPHX[q,p])| - 1)^2 M_2(VPHX[q,p]) \\ &\quad - 2(|V(VPHX[q,p])| - 1) M_1(VPHX[q,p]) F(VPHX[q,p]) \\ &\quad + HM_2(VPHX[q,p]). \end{aligned}$$

And  $M_1(VPHX[q,p]) = 54pq - 10q$ ,  $M_2(VPHX[q,p]) = 81pq + 3q$ , and  $HM_2(VPHX[q,p]) = 9q(81p - 29)$ , given in (Theorem 2.2) above. And since  $F(VPHX[q,p]) = 162pq - 38q$  given in [26] and the partitions of the vertex set and edge set of  $(VPHX[q,p])$  nanotubes are given in (Table 1) respectively [11, 19].

$$\sum |V(VPHX[q,p])| = 6pq, \quad \sum |E(VPHX[q,p])| = 9pq - q$$

Which are complete the proof.

3.3. Second Hyper-Zagreb index of complement V-Phenylenic Nanotorus  $VPHY[m,n]$  ( $\forall m, n \in \mathbb{N} - \{1\}$ )

140 **Corollary 3.3.1** The second Hyper-Zagreb index of complement  $VPHY[m,n]$  nanotorus (Fig 3.) is given by

$$\begin{aligned} HM_2(\overline{VPHY[m,n]}) &= 9mn(6mn - 1)^4 - 108mn(6mn - 1)^3 + 486mn(6mn - 1)^2 \\ &\quad - 17496m^2n^2(6mn - 1) + 729mn. \end{aligned}$$

The edge set of  $VPHY[m,n]$  have only one type of edges:

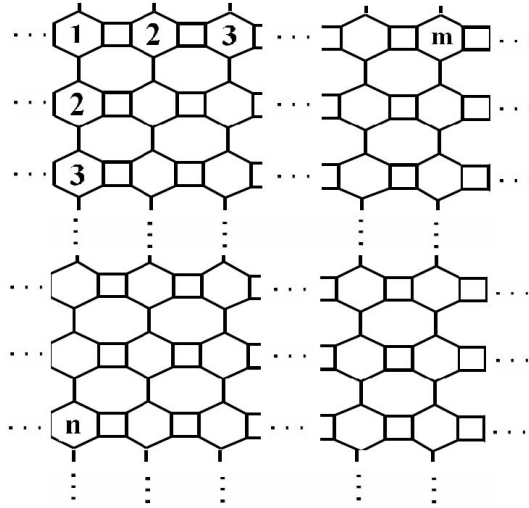


Figure 3: The molecular graph of  $VPHY[m, n]$  nanotorus.

Table 2: The edge and vertex partitions of  $VPHY[m, n]$  nanotorus.

Edge partition	$E_6 = E_9^*$	Vertex partition	$V_3$
Cardinality	$9mn$	Cardinality	$6mn$

$$E_6(VPHY[m, n]) = E_9^* = \{e = uv \in E(VPHY[m, n]) : \delta(u) = 3, \delta(v) = 3\},$$

**Proof.** By using (Theorem 3.1.1) we have

$$\begin{aligned} HM_2(\overline{VPHY[m, n]}) &= |E(VPHY[m, n])|(|V(VPHY[m, n])| - 1)^4 \\ &\quad - 2(|V(VPHY[m, n])| - 1)^3 M_1(VPHY[m, n]) \\ &\quad + (|V(VPHY[m, n])| - 1)^2 F(VPHY[m, n]) \\ &\quad + 4(|V(VPHY[m, n])| - 1)^2 M_2(VPHY[m, n]) \\ &\quad - 2(|V(VPHY[m, n])| - 1) M_1(VPHY[m, n]) F(VPHY[m, n]) \\ &\quad + HM_2(VPHY[m, n]). \end{aligned}$$

And  $M_1(VPHY[m, n]) = 54mn$ ,  $M_2(VPHY[m, n]) = 81mn$ , and  $HM_2(VPHY[m, n]) = 729mn$ , given in (Theorem 2.3) above. And since  $F(VPHY[m, n]) = 162mn$  given in [26] and the partitions of the vertex set and edge set of  $(VPHY[m, n])$  nanotubes are given in (Table 2.) [11, 19].

$$\sum |V(VPHY[m, n])| = 6mn, \quad \sum |E(VPHY[m, n])| = 9mn$$

Which are complete the proof.

#### 145 3.4. Second Hyper-Zagreb index of complement Titania nanotubes and nanotorus

Titania nanotubes are considered 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 [28, 29, 30]. In the following subsection,

150 we study the second Hyper-Zagreb of molecular complement graph Titania nanotubes and molecular complement graph of nanotorus.

**Corollary 3.4.1** The second Hyper-Zagreb index of complement  $TiO_2[n, m]$  nanotube (Fig 4.) is given by

$$\begin{aligned} HM_2(\overline{TiO_2[n, m]}) &= [10mn + 8n][6mn + 6n - 1]^4 \\ &\quad - 2(76mn + 48n)[6mn + 6n - 1]^3 + (840mn + 408n)[6mn + 6n - 1]^2 \\ &\quad + 1930mn + 362n - 2[6mn + 6n - 1](76mn + 48n)(320mn + 160n). \end{aligned}$$

**Proof.** By using (Theorem 3.1.1) we have

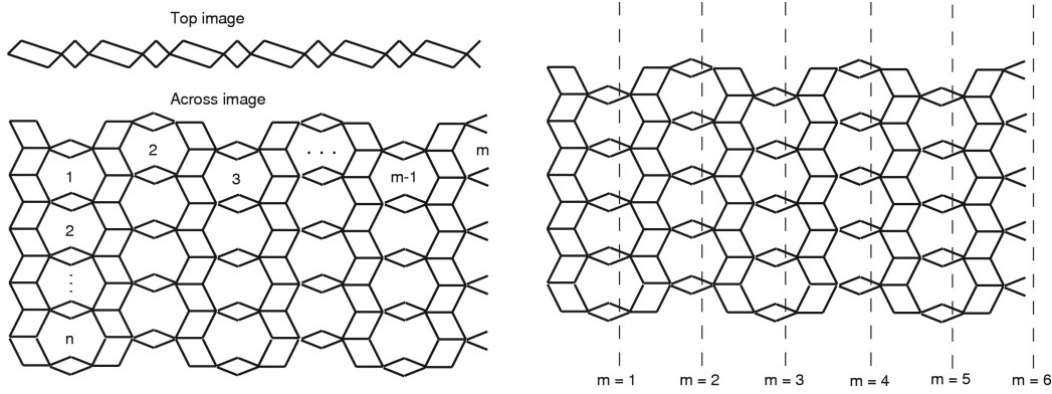


Figure 4: The molecular graph of  $TiO_2[n, m]$  nanotube.

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$$\begin{aligned} HM_2(\overline{TiO_2[n, m]}) &= |E(TiO_2)|(|V(TiO_2)| - 1)^4 - 2(|V(TiO_2)| - 1)^3 M_1(TiO_2) \\ &\quad + (|V(TiO_2)| - 1)^2 F(TiO_2) + 4(|V(TiO_2)| - 1)^2 M_2(TiO_2) \\ &\quad - 2(|V(TiO_2)| - 1) M_1(TiO_2) F(TiO_2) + HM_2(TiO_2). \end{aligned}$$

And since  $M_1(TiO_2[n, m]) = 76mn + 48n$ ,  $M_2(TiO_2[n, m]) = 130mn + 62n$ ,  $F(TiO_2[n, m]) = 320mn + 160n$  given in [28, 29].  $HM_2(TiO_2[n, m]) = 1930mn + 362n$  given in [30]. 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 3,4), respectively. We have

Table 3: 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 4: 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	$6n$	$4mn + 4n$	$6mn - 2n$	$4mn + 2n$	$2n$

$$\begin{aligned}
160 \quad \sum |V(TiO_2[n, m])| &= 6mn + 6n, & \sum |E(TiO_2[n, m])| &= 10mn + 8n \\
HM_2(\overline{TiO_2[n, m]}) &= \sum |E(TiO_2[n, m])| \left[ \sum |V(TiO_2[n, m])| - 1 \right]^4 \\
&- 2M_1(TiO_2) \left[ \sum |V(TiO_2[n, m])| - 1 \right]^3 \\
&+ F(TiO_2) \left[ \sum |V(TiO_2[n, m])| - 1 \right]^2 \\
&+ 4M_2(TiO_2) \left[ \sum |V(TiO_2[n, m])| - 1 \right]^2 \\
&- 2 \left[ \sum |V(TiO_2[n, m])| - 1 \right] M_1(TiO_2) F(TiO_2) + HM_2(TiO_2) \\
&= [|E_8^*| + |E_{10}^* \cup E_{12}^*| + |E_{15}^*|] [6mn + 6n - 1]^4 \\
&- 2(76mn + 48n) [6mn + 6n - 1]^3 + (320mn + 160n) [6mn + 6n - 1]^2 \\
&+ 4(130mn + 62n) [6mn + 6n - 1]^2 + 1930mn + 362n \\
&- 2[6mn + 6n - 1](76mn + 48n)(320mn + 160n) \\
&= [10mn + 8n] [6mn + 6n - 1]^4 \\
&- 2(76mn + 48n) [6mn + 6n - 1]^3 + (840mn + 408n) [6mn + 6n - 1]^2 \\
&+ 1930mn + 362n - 2[6mn + 6n - 1](76mn + 48n)(320mn + 160n).
\end{aligned}$$

**Corollary 3.4.2** Let  $T = T[p, q]$  be the molecular graph of a nanotorus such that  $|V(T)| = pq$ ,  $|E(T)| = \frac{3}{2}pq$  (Fig 5). Then,

- a.  $ReZG_3(T[p, q]) = 81pq$ .
- b.  $HM_2(T[p, q]) = \frac{243}{2}pq$ .
- 165 c.  $HM_2(P_n \times T) = pq[\frac{2837}{2}n - 1831]$ .

**Proof.** To prove identity (a), by definition of redefined third Zagreb index we have

$$ReZG_3(T[p, q]) = \sum_{uv \in E(T[p, q])} \delta_{T[p, q]}(u) \delta_{T[p, q]}(v) [\delta_{T[p, q]}(u) + \delta_{T[p, q]}(v)] = 81pq.$$

To prove identity (b), by definition of second Hyper-Zagreb index we have

$$HM_2(T[p, q]) = \sum_{uv \in E(T[p, q])} [\delta_{T[p, q]}^2(u) \delta_{T[p, q]}^2(v)] = \frac{243}{2}pq.$$

To prove identity (c), by [12] we have

$$\begin{aligned}
HM_2(G_1 \times G_2) &= n_2 HM_2(G_1) + n_1 HM_2(G_2) + 3F(G_1)M_1(G_2) \\
&+ 3F(G_2)M_1(G_1) + m_1[Y(G_2) + 4ReZG_3(G_2)] \\
&+ m_2[Y(G_1) + 4ReZG_3(G_1)] + 4M_1(G_1)M_2(G_2) \\
&+ 4M_1(G_2)M_2(G_1),
\end{aligned}$$

- 170 Where  $M_1(T) = 9pq$ ,  $M_1(P_n) = 4n - 6$ ,  $M_2(T) = 9pq$  and  $M_2(P_n) = 4n - 6$  given in [20].  
 $F(P_n) = 8n - 14$ ,  $F(T) = 27pq$  given in [31].  $ReZG_3(P_n) = 16n - 30$ ,  $ReZG_3(T) = 81pq$

given in identity (b).  $Y(P_n) = 16n - 30$ , given in [8],  $Y(T) = 81pq$ , and since  $HM_2(P_n) = 16n - 40$  given in [12] and  $HM_2(T[p, q]) = \frac{243}{2}pq$  given in identity (b). Then,

$$\begin{aligned}
HM_2(P_n \times T) &= |V(T)|HM_2(P_n) + |V(P_n)|HM_2(T) + 3F(P_n)M_1(T) \\
&+ 3F(T)M_1(P_n) + |E(P_n)|[Y(T) + 4ReZG_3(T)] \\
&+ |E(T)|[Y(P_n) + 4ReZG_3(P_n)] + 4M_1(P_n)M_2(T) \\
&+ 4M_1(T)M_2(P_n) \\
&= pq(16n - 40) + \frac{243}{2}pqn + 27pq(8n - 14) \\
&+ 81pq(4n - 6) + (n - 1)[81pq + 324pq] \\
&+ \frac{3}{2}pq[16n - 30 + 16n - 30] + 36pq(4n - 6) \\
&+ 36pq(4n - 6) \\
&= pq[\frac{2837}{2}n - 1831].
\end{aligned}$$

**Corollary 3.4.3** Let  $T = T[p, q]$  be the molecular graph of a nanotorus such that  $|V(T)| = pq$ ,  $|E(T)| = \frac{3}{2}pq$  (Fig 5.) Then,

$$a. \quad HM_2(\overline{T[p, q]}) = \frac{3}{2}pq(pq - 1)^4 - 18pq(pq - 1)^3 + 81pq(pq - 1)^2 - 486p^2q^2(pq - 1) + \frac{243}{2}pq.$$

$$\begin{aligned}
b. \quad HM_2(\overline{P_n \times T}) &= pq[(npq - 1)^3[\frac{5}{2}n^2pq - npq - \frac{105}{2}n + 37] + (npq - 1)^2[375n - 370] \\
&- 2pq(25n - 18)(npq - 1)(125n - 122) + \frac{2837}{2}n - 1831].
\end{aligned}$$

**Proof.** To prove (a), by using (Theorem 3.1.1) we have

$$\begin{aligned}
HM_2(\overline{T[p, q]}) &= |E(T[p, q])|(|V(T[p, q])| - 1)^4 - 2(|V(T[p, q])| - 1)^3M_1(T[p, q]) \\
&+ (|V(T[p, q])| - 1)^2F(T[p, q]) + 4(|V(T[p, q])| - 1)^2M_2(T[p, q]) \\
&- 2(|V(T[p, q])| - 1)M_1(T[p, q])F(T[p, q]) + HM_2(T[p, q]).
\end{aligned}$$

And since  $M_1(T) = 9pq$ ,  $M_2(T) = \frac{27}{2}pq$  given in [15].  $F(T) = 27pq$  given in [31].  $HM(T[p, q]) = 54pq$  given in [24]. and  $HM_2(T[p, q]) = \frac{243}{2}pq$  given in (Corollary 3.4.2 (b)) above. Then,

$$\begin{aligned}
HM_2(\overline{T[p, q]}) &= |E(T[p, q])|(|V(T[p, q])| - 1)^4 - 2(|V(T[p, q])| - 1)^3M_1(T[p, q]) \\
&+ (|V(T[p, q])| - 1)^2F(T[p, q]) + 4(|V(T[p, q])| - 1)^2M_2(T[p, q]) \\
&- 2(|V(T[p, q])| - 1)M_1(T[p, q])F(T[p, q]) + HM_2(T[p, q]) \\
&= \frac{3}{2}pq(pq - 1)^4 - 18pq(pq - 1)^3 \\
&+ 81pq(pq - 1)^2 - 486p^2q^2(pq - 1) + \frac{243}{2}pq
\end{aligned}$$

To prove (b), since  $M_1(P_n \times T) = pq(25n - 18)$ ,  $M_2(P_n \times T) = \frac{1}{2}pq(125n - 124)$ , given in [23]. and since

$$\begin{aligned}
F(P_n \times T) &= |V(T)|F(P_n) + |V(P_n)|F(T) + 6|E(T)|M_1(P_n) + 6|E(P_n)|M_1(T) \\
&= 2pq(4n - 7) + 27npq + 18pq(2n - 3) + 54pq(n - 1) \\
&= pq[125n - 122].
\end{aligned}$$

By (Corollary 3.4.2 (c))  $HM_2(P_n \times T) = pq[\frac{2837}{2}n - 1831]$  and since  $|E(P_n \times T)| = (n - 1)pq + \frac{3}{2}npq = pq(\frac{5}{2}n - 1)$ ,  $|V(P_n \times T)| = npq$ , and by using (Theorem 3.1.1) we get

$$\begin{aligned}
 HM_2(\overline{P_n \times T}) &= |E(P_n \times T)|(|V(P_n \times T)| - 1)^4 - 2(|V(P_n \times T)| - 1)^3 M_1(P_n \times T) \\
 &+ (|V(P_n \times T)| - 1)^2 F(P_n \times T) + 4(|V(P_n \times T)| - 1)^2 M_2(P_n \times T) \\
 &- 2(|V(P_n \times T)| - 1) M_1(P_n \times T) F(P_n \times T) + HM_2(P_n \times T) \\
 &= pq(\frac{5}{2}n - 1)(npq - 1)^4 - 2pq(npq - 1)^3(25n - 18) \\
 &+ pq[125n - 122](npq - 1)^2 + 2pq(npq - 1)^2(125n - 124) \\
 &- 2p^2q^2(25n - 18)(npq - 1)(125n - 122) + pq[\frac{2837}{2}n - 1831] \\
 &= pq[(npq - 1)^3[\frac{5}{2}n^2pq - npq - \frac{105}{2}n + 37] + (npq - 1)^2[375n - 370] \\
 &- 2pq(25n - 18)(npq - 1)(125n - 122) + \frac{2837}{2}n - 1831].
 \end{aligned}$$

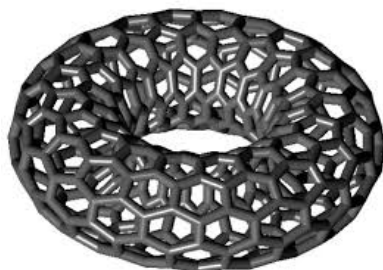


Figure 5: molecular graph of a nanotorus

## 185 Conclusion

This article has presented explicit formulas of some basic mathematical operation for the second Hyper Zagreb index of complement graph operations. Moreover, we computed the second hyper-Zagreb index for some certain important physicochemical structures such as molecular complement graphs of V-Phenylenic Nanotube  $VPHX[q, p]$ , V-Phenylenic Nanotorus  $VPHY[m, n]$  and Titania Nanotubes  $TiO_2$ .

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