The First and Second Zagreb Index of Complement Graph and Its Applications of Molecular Graph

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Authors’ contributions

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Abstract

In this paper, some basic mathematical operation for the second Zagreb indices of graph containing the join and strong product of graph operation, and the first and second Zagreb indices of complement graph 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 $G_1 \ast G_2$ will be explained. The results are applied to molecular graph of nanotorus and titania nanotubes.

Keywords: Zagreb index; Zagreb coindex; complement graph; graph operation.

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1 Introduction

Topological indices are widely used to determine the correlation between the specific properties of molecules and the biological activity with their configuration in the study of quantitative structure-activity relationships (QSARs). In the field of computational chemistry interest in topological indices which capture the structural essence of compounds has been increasing for present time. The interest in topological indices is mainly related to their use in quantitative nonempirical structure-property relationships and quantitative structure-activity relationships [1]. The well-known Zagreb indices introduced in [2],[3] are among the most important topological indices. The first and second Zagreb indices $M_1$ and $M_2$, respectively, are defined for a molecular graph $G$ as:

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

The first and second Zagreb coindices have been introduced by A.R. Ashrafi, T. Doslic, and A. Hamzeh in 2010 [4]. They are respectively defined as:

$$M_1^c(G) = \sum_{uv \notin E(G)} [\delta_C(u) + \delta_C(v)], \quad M_2^c(G) = \sum_{u \in V(G)} \delta_C(u) \delta_C(v),$$

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 $\delta_C(u)$. 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, $uv \notin E(G)$, if and only if $uv \notin E(G)$. Obviously $E(G) \cup E(\overline{G}) = E(K_n)$, and $m = \overline{|E(G)|} = (\frac{n}{2}) - m$, the degree of a vertex $u$ in $\overline{G}$, is the number of edges incident to $u$, denoted by $\delta_{\overline{C}}(u) = n - 1 - \delta_C(u)$. [5],[6].

Then, M. Khalifeh et al.[3] and K. Kiruthika [7] computed the first and second Zagreb indices of 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 $G_1 \ast G_2$ of two graphs. Here we continue this line of research by exploring the behavior of the second Zagreb indices under several important operations such as join and strong product, and studying some basic mathematical operation for the first and second Zagreb indices of complement graphs 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 $G_1 \ast G_2$ of two graphs. 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 their operations [8],[9],[10].

2 Preliminaries

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

Lemma 2.1: [11] 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. $|V(G_1 \times G_2)| = |V(G_1 \circ G_2)| = |V(G_1 \oplus G_2)| = |V(G_1 \ast G_2)| = |V(G_1 \oplus G_2)| = n_1n_2$, $|V(G_1 + G_2)| = n_1 + n_2$.

2. $|E(G_1 \times G_2)| = m_1n_2 + n_1m_2$, $|E(G_1 \circ G_2)| = m_1n_2 + n_1m_2 + 2m_1m_2$, $|E(G_1 \oplus G_2)| = m_1n_2 + n_1m_2$, $|E(G_1 \ast G_2)| = m_1n_2^2 + m_2n_1$, $|E(G_1 \ast G_2)| = m_1n_2^2 + m_2n_1$, $|E(G_1 \ast G_2)| = 2m_1m_2$.
\[E(G_1 \oplus G_2) = m_1n_2^2 + m_2n_1^2 - 4m_1m_2.\]

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

4. \(\delta_{G_1 \oplus 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}.

**Proposition 2.2:**[4] Let \(G\) be a simple graph on \(n\) vertices and \(m\) edges, then
\[
M_1(\overline{G}) = M_1(G) + 2(n-1)(m-n) = n(n-1)^2 - 4m(n-1) + M_1(G), \quad M_1(G) = 2(n-1)m - M_1(\overline{G}).
\]
\[
M_2(\overline{G}) = (n-1)M_1(\overline{G}) + M_2(G) - m(n-1)^2, \quad M_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G).
\]

**Theorem 2.3:**[7] Let \(G_1, G_2\) be two simple graphs with \(n_1, n_2\) vertices and \(m_1, m_2\) edges, respectively, then
\[
M_1(G_1 \oplus G_2) = M_1(G_1) + M_1(G_2) + n_1n_2^2 + n_2n_1^2 + 4m_1n_2 + 4m_2n_1, \quad M_1(G_1 \circ G_2) = M_1(G_1)M_1(G_2).
\]

**Theorem 2.4:**[3] Let \(G_1, G_2\) be two simple graphs with \(n_1, n_2\) vertices and \(m_1, m_2\) edges, respectively, then,
\[
M_1(G_1 \times G_2) = n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2,
\]
\[
M_1(G_1 \circ G_2) = n_2^2M_1(G_1) + n_1M_1(G_2) + 8n_2m_1m_2,
\]
\[
M_1(G_1 \vee G_2) = (n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) + (n_2n_1^2 - 4m_1n_1)M_1(G_2)
+ 8m_1m_2n_1n_2,
\]
\[
M_1(G_1 \oplus G_2) = (n_1n_2^2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2)
+ 8n_1m_2n_1n_2.
\]

**Theorem 2.5:**[7] Let \(G_1, G_2\) be two simple graphs with \(n_1, n_2\) vertices and \(m_1, m_2\) edges, respectively, then
\[
M_2(G_1 \oplus G_2) = 2M_2(G_1)M_2(G_2).
\]

**Theorem 2.6:**[3] Let \(G_1, G_2\) be two simple graphs with \(n_1, n_2\) vertices and \(m_1, m_2\) edges, respectively, then
\[
M_2(G_1 \times G_2) = 3m_1n_2M_1(G_1) + 3m_2n_1M_1(G_2) + n_1M_2(G_2) + n_2M_2(G_1),
\]
\[
M_2(G_1 \circ G_2) = n_2^2M_2(G_1) + n_1M_2(G_2) + 3n_2^2M_2(G_1) + 2n_2m_1M_2(G_2) + 4m_1m_2^2,
\]
\[
M_2(G_1 \vee G_2) = ((n_1^2 - 2m_1^2) - 2n_1^2m_1)M_2(G_2) + ((n_2^2 - 2m_2^2) - 2n_2^2m_2)M_2(G_1)
+ (2m_1n_2m_1 - 4n_1^2m_2)M_1(G_2) + (2n_2^2m_1 - 4n_2^2m_2)M_1(G_1)
- n_1n_2M_1(G_2)M_1(G_1) + 2n_2M_2(G_1)M_1(G_1) + 2n_1M_2(G_2)M_1(G_1)
- 2M_2(G_2)M_2(G_1) + 4m_2m_1(n_2^2m_1 + n_1^2m_2),
\]
\[
M_2(G_1 \oplus G_2) = ((n_1^2 - 2m_1^2) - 4n_1^2m_2)M_2(G_2) + ((n_2^2 - 2m_2^2) - 4n_2^2m_2)M_2(G_1)
+ (2n_1n_2m_1 - 8n_1^2m_2)M_1(G_2) + (2n_2^2m_1 - 8n_2^2m_2)M_1(G_1)
- 2n_1n_2M_1(G_2)M_1(G_1) + 8n_2M_2(G_1)M_1(G_2) + 8n_1M_2(G_2)M_1(G_1)
- 16M_2(G_2)M_2(G_1) + 4m_2m_1(n_2^2m_1 + n_1^2m_2).
\]
3 Main Results

In this section, we study the second Zagreb index of join and strong product of two graphs and the first and second Zagreb index of various complement graph binary operations such as cartesian product, composition, disjunction, symmetric difference, join, tensor product and strong product, of two simple connected graphs. We use the notation $V(G_i)$ for the vertex set, $E(G_i)$, $E(\overline{G_i})$ for the edge set, $n_i$ for the number of vertices and $m_i$, $\overline{m}_i$ for the number of edges of the graph $G_i$, $\overline{G}_i$ respectively. All graphs here offer are simple graphs.

**Proposition 3.1:** Let $G$ be a simple graph on $n$ vertices and $m$ edges, then

$$M_2(G) = \frac{1}{2} n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2.$$  

**Proof.** By using Proposition 2.2, and since $\overline{m} = (\frac{n}{2}) - m$, then

$$M_2(G) = n(n - 1)^3 - 4m(n - 1)^2 + (n - 1)M_1(G) + 2m^2 - M_2(G) - \frac{1}{2} M_1(G)$$

$$(\frac{n}{2}) - m)(n - 1)^2$$

$$= n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - \frac{1}{2} n(n - 1) + 3m(n - 1)^2$$

$$= \frac{1}{2} n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2.$$  

**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 $E(G_1 \otimes G_2) = \{(u_1, v_1)u_1v_1 \in E(G_1) and u_2v_2 \in E(G_2) \}.$

**Theorem 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

$$M_1(G_1 \otimes G_2) = n_1n_2(n_1n_2 - 1)^2 - 8m_1m_2(n_1n_2 - 1) + M_1(G_1)M_1(G_2).$$  

**Proof.** From Proposition 2.2, we have $M_1(G) = n(n - 1)^2 - 4m(n - 1) + M_1(G)$, and since $M_1(G_1 \otimes G_2) = M_1(G_1)M_1(G_2)$, given in Theorem 2.3, and $|E(G_1 \otimes G_2)| = 2m_1m_2$; $|V(G_1 \otimes G_2)| = n_1n_2$ given in Lemma 2.1, then

$$M_1(G_1 \otimes G_2) = |V(G_1 \otimes G_2)|||V(G_1 \otimes G_2)| - 1|^2$$

$$= 4|E(G_1 \otimes G_2)||V(G_1 \otimes G_2)| - 1 + M_1(G_1 \otimes G_2)$$

$$= n_1n_2(n_1n_2 - 1)^2 - 8m_1m_2(n_1n_2 - 1) + M_1(G_1)M_1(G_2).$$  

**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

$$M_2(G_1 \otimes G_2) = \frac{1}{2} n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})M_1(G_1)M_1(G_2)$$

$$+ 8m_1m_2^2 - 2M_2(G_1)M_2(G_2) - 6m_1m_2(n_1n_2 - 1)^2.$$  

**Proof.** From Proposition 3.1, we have $M_2(G) = \frac{1}{2} n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2$, and since $M_1(G_1 \otimes G_2) = M_1(G_1)M_1(G_2)$, $M_2(G_1 \otimes G_2) = 2M_2(G_1)M_2(G_2)$, given in Theorem 2.3 and Theorem 2.5 respectively, and $|E(G_1 \otimes G_2)| = 2m_1m_2$; $|V(G_1 \otimes G_2)| = n_1n_2$.
given in Lemma 2.1. Then.

\[
M_2(G_1 \otimes G_2) = \frac{1}{2} |V(G_1 \otimes G_2)|(|V(G_1 \otimes G_2)| - 1)^3 + (|V(G_1 \otimes G_2)| - \frac{3}{2})M_1(G_1 \otimes G_2)
+ 2|E(G_1 \otimes G_2)| - M_2(G_1 \otimes G_2) - 3|E(G_1 \otimes G_2)|(|V(G_1 \otimes G_2)| - 1)^2
= \frac{1}{2} n_1 n_2 (n_1 n_2 - 1)^3 + (n_1 n_2 - \frac{3}{2})M_1(G_1)M_1(G_2)
+ 8m_1^2 m_2^2 - 2M_2(G_1)M_2(G_2) - 6m_1 m_2 (n_1 n_2 - 1)^2.
\]

**Proof.** From Proposition 2.2, we have \(M_1(G) = n(n - 1)^2 - 4m(n - 1) + M_1(G)\), and since \(M_1(G_1 + G_2) = M_1(G_1) + M_1(G_2) + n_1 n_2 + n_1 n_1 + 4m_1 n_2 + 4m_2 n_1\), given in Theorem 2.3. and \(|E(G_1 + G_2)| = m_1 + m_2 + n_1 n_2\), \(|V(G_1 + G_2)| = n_1 + n_2\) given in Lemma 2.1. Then.

\[
M_1(G_1 \otimes G_2) = |V(G_1 + G_2)|(|V(G_1 + G_2)| - 1)^2
- 4|E(G_1 + G_2)|(|V(G_1 + G_2)| - 1) + M_1(G_1 + G_2)
= (n_1 + n_2)(n_1 + n_2 - 1)^2 - 8(m_1 + m_2 + n_1 n_2)(n_1 + n_2 - 1) + M_1(G_1)
+ M_1(G_2) + n_1 n_2 + n_2 n_1 + 4m_1 n_2 + 4m_2 n_1.
\]

**Theorem 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

\[
M_2(G_1 + G_2) = M_2(G_1) + M_2(G_2) + n_1 M_1(G_1) + n_1 M_1(G_2) + n_1^2 m_1 + n_2^2 m_2
+ 4m_1 m_2 + 2m_1 n_1 n_2 + 2m_2 n_2 n_1 + n_1 n_2.
\]

**Proof.** By Definitions of the second Zagreb index, join \(G_1 + G_2\) and by Lemma 2.1, we have

\[
M_2(G_1 + G_2) = \sum_{u \in E(G_1 + G_2)} \delta_{G_1 + G_2}(u) \delta_{G_1 + G_2}(v)
= \sum_{u \in E(G_1)} \delta_{G_1 + G_2}(u) \delta_{G_1 + G_2}(v) + \sum_{v \in E(G_2)} \delta_{G_1 + G_2}(u) \delta_{G_1 + G_2}(v)
\]
Let $G_1, G_2$ be two simple connected graphs with $n_1, n_2$ vertices and $m_1, m_2$ edges, respectively, then

$$M_2(G_1 + G_2) = \frac{1}{2} n_1 n_2 (n_1 n_2 - 1)^3 + (n_1 n_2 - \frac{3}{2}) |M_1(G_1) + M_1(G_2)| + n_1 n_2^2$$

$$+ n_2 m_1 + 4m_2 n_2 + 4m_2 n_1 + 2|m_1 + m_2 + n_1 n_2|^2 - |M_2(G_1) + M_2(G_2)|$$

$$+ n_2 M_1(G_1) + n_1 M_1(G_2) + n_2^2 m_1 + n_1^2 m_2 + 4m_1 m_2 + 2m_1 n_1 n_2$$

$$+ 2m_2 n_2 n_1 + n_1^2 n_2^2 - 3(m_1 + m_2 + n_1 n_2)(n_1 n_2 - 1)^2.$$
Theorem 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

$$M_1(G_1 \star G_2) = n_1 n_2 (n_1 n_2 - 1)^2 - 4[n_1 n_2 + n_1 m_2 + 2n_2 m_2](n_1 n_2 - 1)$$
$$+ (n_2 + 6m_2)M_1(G_1) + 8m_2 m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2).$$

Proof. From Proposition 2.2, we have $M_1(G) = n(n - 1)^2 - 4m(n - 1) + M_1(G)$, and since $M_1(G_1 \star G_2) = (n_2 + 6m_2)M_1(G_1) + 8m_2 m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)$, given in Proposition 3.7. and $|E(G_1 \star G_2)| = n_1 n_2 + n_1 m_2 + 2m_1 m_2$, $|V(G_1 \star G_2)| = n_1 n_2$ given in Lemma 2.1, then

$$M_1(G_1 \star G_2) = |V(G_1 \star G_2)|(|V(G_1 \star G_2)| - 1)^2$$
$$- 4|E(G_1 \star G_2)|(|V(G_1 \star G_2)| - 1) + M_1(G_1 \star G_2)$$
$$= n_1 n_2 (n_1 n_2 - 1)^2 - 4[n_1 n_2 + n_1 m_2 + 2n_2 m_2](n_1 n_2 - 1)$$
$$+ (n_2 + 6m_2)M_1(G_1) + 8m_2 m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2).$$

Theorem 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

$$M_2(G_1 \star G_2) = (n_2 + 5m_2)M_2(G_1) + (n_1 + 5m_1)M_2(G_2) + 3m_2 P_1(G_1) + 3m_1 P_1(G_2)$$
$$+ 3M_1(G_1)M_1(G_2) + 2M_1(G_2)P_2(G_1) + 2M_1(G_1)P_2(G_2) + M_2(G_1)M_2(G_2).$$

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

$$M_2(G_1 \star G_2) = \sum_{(a,c)(b,d) \in E(G_1 \star G_2)} \delta_{G_1 \star G_2}(a,c) + \delta_{G_1 \star G_2}(b,d)$$
$$= \sum_{a,b \in E(G_1)} \sum_{c,d \in E(G_2)} \delta_{G_1}(a) + \delta_{G_2}(c) + \delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_1}(b) + \delta_{G_2}(d) + \delta_{G_1}(b) \delta_{G_2}(d)$$
$$+ \sum_{a \in E(G_1)} \delta_{G_1}(a) \delta_{G_2}(c) + \delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_1}(b) + \delta_{G_2}(d) + \delta_{G_1}(b) \delta_{G_2}(d)$$
$$= \sum_{a,b \in E(G_1)} \sum_{c,d \in E(G_2)} \delta_{G_1}(a) \delta_{G_2}(c) + \delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_1}(b) + \delta_{G_2}(d) + \delta_{G_1}(b) \delta_{G_2}(d)$$
$$+ \delta_{G_2}(c) \delta_{G_1}(b) + \delta_{G_2}(c) \delta_{G_1}(b) \delta_{G_2}(d) + \delta_{G_2}(c) \delta_{G_1}(b) \delta_{G_2}(d) + \delta_{G_2}(c) \delta_{G_1}(b)$$
$$+ \delta_{G_2}(c) \delta_{G_1}(b) \delta_{G_2}(d) + \delta_{G_2}(c) \delta_{G_1}(b) \delta_{G_2}(d)$$
$$+ \sum_{a \in E(G_1)} \delta_{G_1}(a) \delta_{G_2}(c) + \delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_1}(b) + \delta_{G_2}(d) + \delta_{G_1}(b) \delta_{G_2}(d)$$

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+ \delta_{G_2}(c) \delta_{G_1}(b) + \delta_{G_2}(c) \delta_{G_2}(d) + \delta_{G_2}(c) \delta_{G_1}(b) \delta_{G_2}(d) + \delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_1}(b) \\
+ \sum_{a \in E(G_1)} \sum_{c \in E(G_2)} (\delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_2}(b) + \delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_2}(b) \delta_{G_2}(d) \\
+ \delta_{G_2}(c) \delta_{G_1}(b) + \delta_{G_2}(c) \delta_{G_2}(d) + \delta_{G_2}(c) \delta_{G_1}(b) \delta_{G_2}(d) + \delta_{G_1}(a) \delta_{G_2}(c) \delta_{G_1}(b) \\
= (n_2 + 4m_2)M_2(G_1) + 2m_2M_1(G_1) + m_1M_1(G_2) + M_1(G_2)M_1(G_1) \\
+ M_2(G_1)M_1(G_2) + (n_1 + 4m_1)M_2(G_2) + 2m_1M_1(G_2) + m_2M_1(G_1) \\
+ M_1(G_1)M_1(G_2) + M_2(G_2)M_1(G_1) + m_2M_2(G_1) + M_1(G_1)M_2(G_2) \\
+ m_1M_2(G_2) + M_1(G_1)M_2(G_2) + M_1(G_1)M_2(G_2) + M_2(G_1)M_2(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_1(G_1) + 2M_1(G_1)M_2(G_2) + M_2(G_1)M_2(G_2).

**Theorem 3.10:** Let $G_1$, $G_2$ be two simple connected graphs with $n_1$, $n_2$ vertices and $m_1$, $m_2$ edges, respectively, then

$$M_2(G_1 \ast G_2) = \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[(n_2 + 6m_2)M_1(G_1) + 8m_2m_1 \\
+ (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)] + 2m_1n_2 + n_1m_2 + 2m_1m_2^2 \\
- [(n_2 + 5m_2)M_2(G_2) + (n_1 + 5m_1)M_2(G_1) + 3m_2M_1(G_1) + 3m_1M_1(G_2) \\
+ 3M_1(G_1)M_2(G_2) + 2M_1(G_2)M_2(G_1) + M_2(G_1)M_2(G_2) + M_2(G_2)M_2(G_2)] \\
- 3(m_1n_2 + n_1m_2 + 2m_1m_2)(n_1n_2 - 1)^2. $$

**Proof.** From Proposition 3.1, we have $M_2(G_1) = \frac{1}{2}(n(n-1)^3 + (n-\frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, and since $M_1(G_1 \ast G_2) = (n_2 + 6m_2)M_1(G_1) + 8m_2m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)$, given in Proposition 3.7. $M_2(G_1 \ast G_2) = (n_2 + 5m_2)M_2(G_1) + (n_1 + 5m_1)M_2(G_2) + 3m_2M_1(G_1) + 3m_1M_1(G_2) + 3M_1(G_1)M_1(G_2) + 2M_1(G_2)M_1(G_1) + 2M_1(G_1)M_2(G_2) + M_2(G_1)M_2(G_2)$, given in Theorem 3.9. and $|E(G_1 \ast G_2)| = m_1n_2 + n_1m_2 + 2m_1m_2$, $|V(G_1 \ast G_2)| = n_1n_2$ given in Lemma 2.1. Then,

$$M_2(G_1 \ast G_2) = \frac{1}{2}|V(G_1 \ast G_2)|(|V(G_1 \ast G_2)| - 1)^3 + |V(G_1 \ast G_2)| - \frac{3}{2}M_1(G_1 \ast G_2) \\
+ 2|E(G_1 \ast G_2)|^2 - M_2(G_1 \ast G_2) - 3|E(G_1 \ast G_2)|(|V(G_1 \ast G_2)| - 1)^2 \\
= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[(n_2 + 6m_2)M_1(G_1) + 8m_2m_1 \\
+ (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)] + 2m_1n_2 + n_1m_2 + 2m_1m_2^2 \\
- [(n_2 + 5m_2)M_2(G_2) + (n_1 + 5m_1)M_2(G_1) + 3m_2M_1(G_1) + 3m_1M_1(G_2) \\
+ 3M_1(G_1)M_2(G_2) + 2M_1(G_2)M_2(G_1) + M_2(G_1)M_2(G_2) + M_2(G_1)M_2(G_2)] \\
- 3(m_1n_2 + n_1m_2 + 2m_1m_2)(n_1n_2 - 1)^2. $$

**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 $x = y$.

**Theorem 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

$$M_1(G_1 \times G_2) = n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2 + n_1m_2)(n_1n_2 - 1) + n_2M_1(G_1) \\
+ n_1M_1(G_2) + 8m_1m_2.$$
Proof. From Proposition 2.2, we have \( M_1(G) = n(n - 1)^2 - 4m(n - 1) + M_1(G) \), and since \( M_1(G_1 \times G_2) = n_2 M_1(G_1) + n_1 M_1(G_2) + 8m_1 m_2 \), given in Theorem 2.4. and \( |E(G_1 \times G_2)| = n_1 n_2 + n_1 m_2 \), \(|V(G_1 \times G_2)| = n_1 n_2\) given in Lemma 2.1. Then
\[
\begin{align*}
M_1(G_1 \times G_2) &= |V(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1)^2 \\
&= n_1 n_2 (n_1 n_2 - 1)^2 - 4(n_1 n_2 + n_1 m_2)(n_1 n_2 - 1) + n_2 M_1(G_1) \\
&+ n_1 M_1(G_2) + 8m_1 m_2.
\end{align*}
\]

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
\[
\begin{align*}
M_2(G_1 \times G_2) &= \frac{1}{2}n_1 n_2 (n_1 n_2 - 1)^3 + (n_1 n_2 - \frac{3}{2})n_2 M_1(G_1) + n_1 M_1(G_2) + 8m_1 m_2 \\
&+ 2[n_1 n_2 + n_1 m_2]^2 - [3m_2 M_1(G_1) + 3m_1 M_1(G_2) + n_1 M_2(G_2) + n_2 M_2(G_1)] \\
&- 3(m_1 n_2 + n_1 m_2)(n_1 n_2 - 1)^2.
\end{align*}
\]

Proof. From Proposition 3.1, we have \( M_2(G) = \frac{1}{2}n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2 \), and since \( M_1(G_1 \times G_2) = n_2 M_1(G_1) + n_1 M_1(G_2) + 8m_1 m_2 \), \( M_2(G_1 \times G_2) = 3m_2 M_1(G_1) + 3m_1 M_1(G_2) + n_1 M_2(G_2) + n_2 M_2(G_1) \), given in Theorem 2.4. and Theorem 2.6. respectively, and
\[
|E(G_1 \times G_2)| = n_1 n_2 + n_1 m_2, \quad |V(G_1 \times G_2)| = n_1 n_2 \text{ given in Lemma 2.1. Then}
\begin{align*}
M_2(G_1 \times G_2) &= \frac{1}{2}|V(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1)^3 + |V(G_1 \times G_2)| - \frac{3}{2}M_1(G_1 \times G_2) \\
&+ 2[E(G_1 \times G_2)]^2 - M_2(G_1 \times G_2) - 3|E(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1)^2 \\
&= \frac{1}{2}n_1 n_2 (n_1 n_2 - 1)^3 + (n_1 n_2 - \frac{3}{2})n_2 M_1(G_1) + n_1 M_1(G_2) + 8m_1 m_2 \\
&+ 2[n_1 n_2 + n_1 m_2]^2 - [3m_2 M_1(G_1) + 3m_1 M_1(G_2) + n_1 M_2(G_2) + n_2 M_2(G_1)] \\
&- 3(m_1 n_2 + n_1 m_2)(n_1 n_2 - 1)^2.
\end{align*}
\]

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 \( (u_1, u_2) \) is adjacent with \( v_1, v_2 \).

Theorem 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
\[
\begin{align*}
M_1(G_1 \circ G_2) &= n_1 n_2 (n_1 n_2 - 1)^2 - 4(m_1 n_2^2 + m_2 n_1)(n_1 n_2 - 1) + n_2^3 M_1(G_1) \\
&+ n_1 M_1(G_2) + 8n_2 m_2 m_1.
\end{align*}
\]

Proof. From Proposition 2.2, we have \( M_1(G) = n(n - 1)^2 - 4m(n - 1) + M_1(G) \), and since \( M_1(G_1 \circ G_2) = n_2^2 M_1(G_1) + n_1 M_1(G_2) + 8n_2 m_2 m_1 \), given in Theorem 2.4. and \( |E(G_1 \circ G_2)| = n_1 n_2 + n_1 m_2 \), \(|V(G_1 \circ G_2)| = n_1 n_2\) given in Lemma 2.1. Then
\[
\begin{align*}
M_1(G_1 \circ G_2) &= |V(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1)^2 \\
&= n_1 n_2 (n_1 n_2 - 1)^2 - 4(m_1 n_2^2 + m_2 n_1)(n_1 n_2 - 1) + n_2^3 M_1(G_1) \\
&+ n_1 M_1(G_2) + 8n_2 m_2 m_1.
\end{align*}
\]
Theorem 3.14: Let $G_1, G_2$ be two simple connected graphs with $n_1, n_2$ vertices and $m_1, m_2$ edges, respectively, then

$$M_2(G_1 \cup G_2) = \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[n_2^2M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1] + 2[n_1n_2^2 + m_2n_1]^2 - [n_2^2M_2(G_1) + n_1M_2(G_2) + 3n_2m_2M_2(G_1)] + 2n_2m_1M_1(G_2) + 4m_1m_2^2] - 3(m_1n_2^2 + m_2n_1)(n_1n_2 - 1)^2.$$

Proof. From Proposition 3.1, we have $M_2(G) = \frac{1}{4}n(n-1)^2 + (n-\frac{1}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, and since $M_1(G_1 \circ G_2) = n_2^2M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1$, $M_2(G_1 \circ G_2) = n_2^4M_2(G_1) + n_1M_2(G_2) + 3n_2m_2M_2(G_1) + 2n_2m_1M_1(G_2) + 4m_1m_2^2$, given in Theorem 2.4. and Theorem 2.6. respectively, and $|E(G_1 \circ G_2)| = m_1n_2^2 + m_2n_1$, $|V(G_1 \circ G_2)| = n_1n_2$ given in Lemma 2.1. Then.

$$M_2(G_1 \circ G_2) = \frac{1}{2}|V(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1)^3 + (|V(G_1 \circ G_2)| - \frac{3}{2})M_1(G_1 \circ G_2) + 2|E(G_1 \circ G_2)|^2 - M_2(G_1 \circ G_2) - 3|E(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1)^2 = \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[n_2^2M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1] + 2[n_1n_2^2 + m_2n_1]^2 - [n_2^2M_2(G_1) + n_1M_2(G_2) + 3n_2m_2M_2(G_1)] + 2n_2m_1M_1(G_2) + 4m_1m_2^2] - 3(m_1n_2^2 + m_2n_1)(n_1n_2 - 1)^2.$$

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 to $(u_2, v_2)$, whenever $(u_1, u_2) \in E(G_1)$ or $(v_1, v_2) \in E(G_2)$.

Theorem 3.15: Let $G_1, G_2$ be two simple connected graphs with $n_1, n_2$ vertices and $m_1, m_2$ edges, respectively, then

$$M_1(G_1 \vee G_2) = n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1^2 - 2m_1m_2)(n_1n_2 - 1) + (n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) + (n_2n_1^2 - 4m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2.$$

Proof. From Proposition 2.2, we have $M_1(\overline{G}) = (n-1)^2 + 4m(n-1) + M_1(G)$, and since $M_1(G_1 \vee G_2) = (n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) + (n_2n_1^2 - 4m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2$ given in Theorem 2.4. and $|E(G_1 \vee G_2)| = m_1n_2^2 + m_2n_1^2 - 2m_1m_2$, $|V(G_1 \vee G_2)| = n_1n_2$ given in Lemma 2.1. Then.

$$M_1(G_1 \vee G_2) = |V(G_1 \vee G_2)|(|V(G_1 \vee G_2)| - 1)^2 - 4|E(G_1 \vee G_2)|(|V(G_1 \vee G_2)| - 1) + M_1(G_1 \vee G_2) = n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1^2 - 2m_1m_2)(n_1n_2 - 1) + (n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) + (n_2n_1^2 - 4m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2.$$

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Theorem 3.16: Let $G_1$, $G_2$ be two simple connected graphs with $n_1$, $n_2$ vertices and $m_1$, $m_2$ edges, respectively, then
\[
M_2(G_1 \lor G_2) = \frac{1}{2} n_1 n_2 (n_1 n_2 - 1)^3 + (n_1 n_2 - 3) [((n_1^2 - 4) m_1 n_2 - 4 m_2 n_2) M_1(G_1) + M_1(G_2) M_1(G_1)] \\
+ (n_1^2 - 4 m_1 n_1) M_1(G_2) + 8 m_1 m_2 n_1 n_2 + 2 [m_1 n_2^2 + m_2 n_1^2 - 2 m_1 m_2]^2 \\
- [(n_1^2 - 2 m_1)^2 - 2 n_1^2 m_1) M_2(G_2) + ((n_1^2 - 2 m_2)^2 - 2 n_2^2 m_2) M_2(G_1)] \\
+ (2 n_1^2 m_2 - 4 m_2^2) M_1(G_2) + 2 n_1 M_2(G_2) M_1(G_1) - 2 M_2(G_2) M_1(G_1) \\
+ 2 n_2 M_2(G_1) M_1(G_2) + (2 n_2^2 m_2 - 4 m_2^2) M_1(G_1) - n_1 n_2 M_1(G_2) M_1(G_1) \\
+ 4 m_2 m_1 (n_2^2 m_1 + n_1^2 m_2)] - 3 [m_1 n_2^2 + m_2 n_1^2 - 2 m_1 m_2] (n_1 n_2 - 1)^2.
\]

Proof. From Proposition 3.1.
\[
M_2(G) = \frac{1}{2} n(n - 1)^3 + (n - \frac{3}{2}) M_1(G) + 2 m^2 - M_2(G) - 3(m(n - 1)^2, \text{ and by Theorem 2.4. and Theorem 2.6. respectively, we have}
\]
\[
M_1(G_1 \lor G_2) = (n_1 n_2^2 - 4 m_2 n_1) M_1(G_1) + M_1(G_2) M_1(G_1) + (n_2 n_2^2 - 4 m_1 n_2) M_1(G_2) \\
+ 8 m_1 m_2 n_1 n_2,
\]
\[
M_2(G_1 \lor G_2) = (n_1^2 - 2 m_1)^2 - 2 n_1^2 m_1) M_2(G_2) + ((n_2^2 - 2 m_2)^2 - 2 n_2^2 m_2) M_2(G_1) \\
+ (2 n_1^2 m_2 - 4 m_2^2) M_1(G_2) + 2 n_1 M_2(G_2) M_1(G_1) - 2 M_2(G_2) M_1(G_1) \\
- n_1 n_2 M_1(G_2) M_1(G_1) + 2 n_2 M_2(G_1) M_1(G_2) + 2 n_2 M_1(G_2) M_1(G_1) \\
- 2 M_2(G_2) M_2(G_1) + 4 m_2 m_1 (n_2^2 m_1 + n_1^2 m_2),
\]
and since $|E(G_1 \lor G_2)| = m_1 n_2^2 + m_2 n_1^2 - 2 m_1 m_2$, $|V(G_1 \lor G_2)| = n_1 n_2$ given in Lemma 2.1. Then.
\[
M_2(G_1 \lor G_2) = \frac{1}{2} |V(G_1 \lor G_2)| |V(G_1 \lor G_2)| - (n_1 n_2 - 1)^3 + (n_1 n_2 - 3) [((n_1^2 - 2 m_1)^2 - 2 n_1^2 m_1) M_2(G_2) + ((n_2^2 - 2 m_2)^2 - 2 n_2^2 m_2) M_2(G_1)] \\
+ (2 n_1^2 m_2 - 4 m_2^2) M_1(G_2) + 2 n_1 M_2(G_2) M_1(G_1) - 2 M_2(G_2) M_1(G_1) \\
+ (2 n_2 M_2(G_1) M_1(G_2) + (2 n_2^2 m_2 - 4 m_2^2) M_1(G_1) - n_1 n_2 M_1(G_2) M_1(G_1) \\
+ 4 m_2 m_1 (n_2^2 m_1 + n_1^2 m_2)] - 3 [m_1 n_2^2 + m_2 n_1^2 - 2 m_1 m_2] (n_1 n_2 - 1)^2.
\]

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 $E(G_1 \oplus G_2) = \{(u_1, u_2)(v_1, v_2)|u_1 v_1 \in E(G_1) \text{ or } u_2 v_2 \in E(G_2) \}$ but not both.

Theorem 3.17: Let $G_1$, $G_2$ be two simple connected graphs with $n_1$, $n_2$ vertices and $m_1$, $m_2$ edges, respectively, then
\[
M_1(G_1 \oplus G_2) = n_1 n_2 (n_1 n_2 - 1)^2 - 4 m_1 n_2^2 + m_2 n_1^2 - 4 m_1 m_2 (n_1 n_2 - 1) \\
+ (n_1 n_2^2 - 8 m_2 n_1) M_1(G_1) + 4 M_1(G_1) M_1(G_2) + (n_2 n_1^2 - 8 m_1 n_2) M_1(G_2) \\
+ 8 m_1 m_2 n_1 n_2.
\]
Proof. From Proposition 2.2, we have $M_1(G) = n(n-1)^2 - 4m(n-1) + M_1(G)$, and since $M_1(G_1 \oplus G_2) = (n_1n_2^2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2$, given in Theorem 2.4, and $|E(G_1 \oplus G_2)| = m_1n_2^2 + m_2n_1^2 - 4m_1m_2$, $|V(G_1 \oplus G_2)| = n_1n_2$ given in Lemma 2.1. Then,

$$M_1(G_1 \oplus G_2) = |V(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)^2 - 4|E(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)$$

$$+ M_1(G_1 \oplus G_2) = n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1^2 - 4m_1m_2)(n_1n_2 - 1)$$

$$+ (n_2n_1^2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2.$$ 

Theorem 3.18: Let $G_1, G_2$ be two simple connected graphs with $n_1, n_2$ vertices and $m_1, m_2$ edges, respectively, then

$$M_2(G_1 \oplus G_2) = 12n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - 3/2)2(m_1n_2 - 8m_2n_2)M_1(G_1)$$

$$+ 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2$$

$$+ 2(m_1n_2^2 + m_2n_1^2 - 4m_1m_2) + (((n_1^2 - 2m_1)^2 - 4m_1^2)M_2(G_2)$$

$$+ ((n_2^2 - 2m_2)^2 - 4m_2^2)M_2(G_2) + 2n_2m_1^2 - 8m_1^2)M_1(G_1)$$

$$+ (2n_2m_1 - m_2)M_1(G_2) + 8m_2M_1(G_2) + 16M_2(G_2) + 4m_2m_1(n_2m_1 + n_1m_2).$$

and since $|E(G_1 \oplus G_2)| = m_1n_2^2 + m_2n_1^2 - 4m_1m_2$, $|V(G_1 \oplus G_2)| = n_1n_2$ given in Lemma 2.1. Then,

$$M_2(G_1 \oplus G_2) = (n_1n_2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2)$$

$$+ 8m_1m_2n_1n_2.$$ 

Proof. From Proposition 3.1, $M_2(G) = 12(n(n-1)^3 + (n - 4/2)m_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, and by Theorem 2.4, and Theorem 2.6, respectively, we have

$$M_1(G_1 \oplus G_2) = (n_1n_2^2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2)$$

$$+ 8m_1m_2n_1n_2.$$ 

and since $|E(G_1 \oplus G_2)| = m_1n_2^2 + m_2n_1^2 - 4m_1m_2$, $|V(G_1 \oplus G_2)| = n_1n_2$ given in Lemma 2.1. Then,

$$M_2(G_1 \oplus G_2) = (n_1n_2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2)$$

$$+ 8m_1m_2n_1n_2.$$ 

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4 Application

In this section, first and second Zagreb index have been investigated for complement titania $\text{TiO}_2$ nanotubes and molecular graph of nanotorus.

Corollary 4.1: The first and second Zagreb index of complement $\text{TiO}_2[n,m]$ nanotube Fig. 1. is given by

- **a.** $M_1(\overline{\text{TiO}_2[n,m]}) = 2n(6mn + 6n - 1)[18mn(m + 1) + 18n - 23m - 19] + 4n(19m + 12)$,
- **b.** $M_2(\overline{\text{TiO}_2[n,m]})$
  \[= 3n(m+1)(6mn + 6n - 1)^3 + 4n(6mn + 6n - \frac{3}{2})(19m + 12) + 4n(5m + 4)[(10mn + 8n) - 3(6mn + 6n - 1)^2] - 2n(65m + 31).\]

![Fig. 1. The molecular graph of $\text{TiO}_2[n,m]$ nanotube](image)

**Proof.** Proving item (a) by Proposition 2.2 we have

\[M_1(\overline{G}) = n(n - 1)^2 - 4m(n - 1) + M_1(G),\]

and since $M_1(\text{TiO}_2[n,m]) = 76mn + 48n$, and the partitions of the vertex set and edge set $\sum |V(\text{TiO}_2[n,m])| = 6mn + 6n$, $\sum |E(\text{TiO}_2[n,m])| = 10mn + 8n$ of titania nanotubes are given in [13, 14]. Then

\[M_1(\overline{\text{TiO}_2[n,m]}) = \sum |V(\text{TiO}_2[n,m])|(\sum |V(\text{TiO}_2[n,m])| - 1)^2 - 4 \sum |E(\text{TiO}_2[n,m])|(\sum |V(\text{TiO}_2[n,m])| - 1) + M_1(\text{TiO}_2[n,m]) = 2n(6mn + 6n - 1)[18mn(m + 1) + 18n - 23m - 19] + 4n(19m + 12).\]

Proving item (b) by Proposition 3.1 we have

\[M_2(\overline{G}) = \frac{1}{3}n(n - 1)^3 + (n - \frac{2}{3})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2,\]

and since $M_1(\text{TiO}_2[n,m]) = 76mn + 48n$, $M_2(\text{TiO}_2[n,m]) = 130mn + 62n$ and the partitions of the vertex set and edge set $\sum |V(\text{TiO}_2[n,m])| = 6mn + 6n$, $\sum |E(\text{TiO}_2[n,m])| = 10mn + 8n$ of titania nanotubes
are given in [14]. Hence

\[
M_2(T[iO_2[n, m]]) = \frac{1}{2} \sum |V(T[iO_2[n, m])|\sum |V(T[iO_2[n, m])| - 1)^3
+ (\sum |V(T[iO_2[n, m])| - \frac{3}{2})M_1(T[iO_2[n, m])
+ 2|E(T[iO_2[n, m])| - M_2(T[iO_2[n, m])
- 3|E(T[iO_2[n, m])|\sum |V(T[iO_2[n, m])| - 1)^2
= \frac{1}{2}(6mn + 6n)(6mn + 6n - 1)^3 + (6mn + 6n - \frac{3}{2})(76mn + 48n)
+ 2|10mn + 8n|^2 - 130mn - 62n - 3(10mn + 8n)(6mn + 6n - 1)^2
+ 3n(m + 1)(6mn + 6n - 1)^3 + 4n(6mn + 6n - \frac{3}{2})(19m + 12)
+ 4n(5m + 4)(10mn + 8n) - 3(6mn + 6n - 1)^2 - 2n(65m + 31).
\]

**Corollary 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. 2. Then:

\( a. \) \( M_1(T[p, q]) = pq[p^2q^2 - 8pq + 16]. \)

\( b. \) \( M_1(T_n \times T) = pq[n^3p^2q^2 - 12n^2pq + 4npq + 36n - 22]. \)

\( c. \) \( M_2(T[p, q]) = pq[\frac{1}{2}(pq - 1)^2(pq - \frac{11}{2}) + \frac{27}{2}pq - 27]. \)

\( d. \) \( M_2(T_n \times T) = pq[\frac{1}{2}n(npq - 1)^3 + (npq - \frac{3}{2})(25n - 18) + 2pq(\frac{5}{2}n - 1)^2 - \frac{1}{2}(125n - 124)
- 3(\frac{5}{2}n - 1)(npq - 1)^2]. \)

**Proof.** Proving item (a) by Proposition 2.2 we have \( M_1(G) = n(n - 1)^2 - 4m(n - 1) + M_1(G) \), and since \( M_1(T) = 9pq \) given in [3]. Then

\[
M_1(T[p, q]) = |V(T)|||V(T)| - 1)^2 - 4|E(T)|||V(T)| - 1) + M_1(T)
= pq(pq - 1)^2 - \frac{3}{2}pq(pq - 1) + 9pq
= pq[p^2q^2 - 8pq + 16].
\]

Proving item (b) by [3] \( M_1(P_n \times T) = pq(25n - 18) \), and by using Lemma 2.1. \( |E(P_n \times T)| = pq(\frac{5}{2}n - 1) \), \( |V(P_n \times T)| = npq \), and by using Proposition 2.2. we get

\[
M_1(P_n \times T) = |V(P_n \times T)|||V(P_n \times T)| - 1)^2 - 4|E(P_n \times T)|||V(P_n \times T)| - 1) + M_1(P_n \times T)
= npq(npq - 1)^2 - 4pq(\frac{5}{2}n - 1)(npq - 1) + pq(25n - 18)
= pq[n^3p^2q^2 - 12n^2pq + 4npq + 36n - 22].
\]
Proving item (c) by Proposition 3.1. we have \( M_2(T) = \frac{1}{2} n(n-1)^3 + (n-\frac{1}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2 \), and since \( M_1(T) = 9pq, M_2(T) = \frac{27}{2}pq \) given in [3]. Then

\[
M_2(T[p, q]) = \frac{1}{2} |V(T)|(|V(T)| - 1)^3 + (|V(T)| - \frac{3}{2})M_1(T) + 2|E(T)|^2 - M_2(T) - 3|E(T)||V(T)| - 1)^2
\]

\[
= \frac{1}{2} pq(pq - 1)^3 + 9pq(pq - \frac{3}{2}) + 2\left(\frac{3}{2}pq\right)^2 - 27 pq - 3\left(\frac{3}{2}pq(pq - 1)^2
\]

\[
= pq\left(\frac{1}{2}(pq - \frac{11}{2}) + \frac{27}{2}pq - 27\right).
\]

Proving item (d) by [3] \( M_1(P_n \times T) = pq(25n - 18), M_2(P_n \times T) = \frac{1}{2}pq(125n - 124) \), and by using Lemma 2.1. \( |E(P_n \times T)| = pq\left(\frac{5}{2}n - 1\right), |V(P_n \times T)| = npq \), and by using Proposition 3.1. we get

\[
M_2(P_n \times T) = \frac{1}{2}|V(P_n \times T)|(|V(P_n \times T)| - 1)^3 + (|V(P_n \times T)| - \frac{3}{2})M_1(P_n \times T)
+ 2|E(P_n \times T)|^2 - M_2(P_n \times T) - 3|E(P_n \times T)|(|V(P_n \times T)| - 1)^2
\]

\[
= pq\left(\frac{1}{2}n(npq - 1)^3 + (npq - \frac{3}{2})(25n - 18) + 2pq\right)\left(\frac{5}{2}n - 1\right)^2
\]

\[
- \frac{1}{2}(125n - 124) - 3\left(\frac{5}{2}n - 1\right)(npq - 1)^2.
\]

Fig. 2. Molecular graph of a nanotorus

5 Conclusion

We studied the second Zagreb index of join and strong product of two graphs and the first and second Zagreb index of various complement graph binary operations such as Cartesian product, composition, disjunction, symmetric difference, join, tensor product and strong product, of two simple connected graphs. Moreover we calculated the first and second-Zagreb index of molecular complement graph of nanotorus and titania nanotubes \( TiO_2[n, m] \).

Competing Interests

Authors have declared that no competing interests exist.
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