

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

Mohammed S. Alsharafi^{1*}, Mahioub M. Shubatah²
and Abdu Q. Alameri³

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

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

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

Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/AJPAS/2020/v8i330207

Editor(s):

(1) Dr. Manuel Alberto M. Ferreira, Lisbon University, Portugal.

Reviewers:

(1) Simge Öztunç, Manisa Celal Bayar University, Turkey.

(2) Chacha Stephen, Mkwawa University College of Education, Tanzania.

(3) M. Felix Nes Mabel, St. Xavier's Catholic College of Engineering, India.

Complete Peer review History: <http://www.sdiarticle4.com/review-history/60364>

Received: 12 June 2020

Accepted: 17 August 2020

Published: 22 August 2020

Original Research Article

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 $\overline{G_1} \times \overline{G_2}$, composition $\overline{G_1} \circ \overline{G_2}$, disjunction $\overline{G_1} \vee \overline{G_2}$, symmetric difference $\overline{G_1} \oplus \overline{G_2}$, join $\overline{G_1} + \overline{G_2}$, tensor product $\overline{G_1} \otimes \overline{G_2}$, and strong product $\overline{G_1} * \overline{G_2}$ will be explained. The results are applied to molecular graph of nanotorus and titania nanotubes.

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

*Corresponding author: E-mail: alsharafi205010@gmail.com;

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:

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

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

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

Throughout this paper, we consider a finite connected graph G that has no loops or multiple edges with vertex and edge sets $V(G)$, and $E(G)$, respectively. For a graph G , the degree of a vertex u is the number of edges incident to u , denoted by $\delta_G(u)$. The complement of G , denoted by \overline{G} , is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent, i.e., connected by an edge uv , if and only if they are not adjacent in G . Hence, $uv \in E(\overline{G})$, if and only if $uv \notin E(G)$. Obviously $E(G) \cup E(\overline{G}) = E(K_n)$, and $\overline{m} = |E(\overline{G})| = \binom{n}{2} - m$, the degree of a vertex u in \overline{G} , is the number of edges incident to u , denoted by $\delta_{\overline{G}}(u) = n - 1 - \delta_G(u)$, [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 $G_1 * G_2$ 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 $\overline{G_1} \times \overline{G_2}$, composition $\overline{G_1} \circ \overline{G_2}$, disjunction $\overline{G_1} \vee \overline{G_2}$, symmetric difference $\overline{G_1} \oplus \overline{G_2}$, join $\overline{G_1} + \overline{G_2}$, tensor product $\overline{G_1} \otimes \overline{G_2}$, and strong product $\overline{G_1} * \overline{G_2}$ 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

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

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

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

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

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

3. $\delta_{G_1 * G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v) + \delta_{G_1}(u)\delta_{G_2}(v),$
4. $\delta_{G_1 + G_2}(a) = \begin{cases} \delta_{G_1}(a) + n_2 & a \in V(G_1) \\ \delta_{G_2}(a) + n_1 & a \in V(G_2) \end{cases}.$

Proposition 2.2:[4] Let G be a simple graph on n vertices and m edges, then

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

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

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

$$M_1(G_1 + G_2) = M_1(G_1) + M_1(G_2) + n_1 n_2^2 + n_2 n_1^2 + 4m_1 n_2 + 4m_2 n_1, \quad M_1(G_1 \otimes G_2) = M_1(G_1)M_1(G_2).$$

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.

$$M_1(G_1 \times G_2) = n_2 M_1(G_1) + n_1 M_1(G_2) + 8m_1 m_2,$$

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

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

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

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

$$M_2(G_1 \otimes G_2) = 2M_2(G_1)M_2(G_2).$$

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

$$M_2(G_1 \times G_2) = 3m_2 M_1(G_1) + 3m_1 M_1(G_2) + n_1 M_2(G_2) + n_2 M_2(G_1),$$

$$M_2(G_1 \circ G_2) = n_2^4 M_2(G_1) + n_1 M_2(G_2) + 3n_2^2 m_2 M_1(G_1) + 2n_2 m_1 M_1(G_2) + 4m_1 m_2^2,$$

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

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

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

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

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

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

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 $E(G_1 \otimes G_2) = (u_1, u_2)(v_1, v_2) | u_1v_1 \in E(G_1) \text{ and } u_2v_2 \in E(G_2)$.

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

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

Proof. From Proposition 2.2. we have $M_1(\overline{G}) = n(n-1)^2 - 4m(n-1) + M_1(G)$, 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

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

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

$$\begin{aligned} M_2(\overline{G_1 \otimes G_2}) &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})M_1(G_1)M_1(G_2) \\ &+ 8m_1^2m_2^2 - 2M_2(G_1)M_2(G_2) - 6m_1m_2(n_1n_2 - 1)^2. \end{aligned}$$

Proof. From Proposition 3.1. we have $M_2(\overline{G}) = \frac{1}{2}n(n-1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, 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.

$$\begin{aligned}
 M_2(\overline{G_1 \otimes G_2}) &= \frac{1}{2}|V(G_1 \otimes G_2)|(|V(G_1 \otimes G_2)| - 1)^3 + (|V(G_1 \otimes G_2)| - \frac{3}{2})M_1(G_1 \otimes G_2) \\
 &+ 2|E(G_1 \otimes G_2)|^2 - M_2(G_1 \otimes G_2) - 3|E(G_1 \otimes G_2)|(|V(G_1 \otimes G_2)| - 1)^2 \\
 &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})M_1(G_1)M_1(G_2) \\
 &+ 8m_1^2m_2^2 - 2M_2(G_1)M_2(G_2) - 6m_1m_2(n_1n_2 - 1)^2.
 \end{aligned}$$

Join

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

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

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

Proof. From Proposition 2.2. we have $M_1(\overline{G}) = n(n - 1)^2 - 4m(n - 1) + M_1(G)$, and since $M_1(G_1 + G_2) = M_1(G_1) + M_1(G_2) + n_1n_2^2 + n_2n_1^2 + 4m_1n_2 + 4m_2n_1$, given in Theorem 2.3. and $|E(G_1 + G_2)| = m_1 + m_2 + n_1n_2$, $|V(G_1 + G_2)| = n_1 + n_2$ given in Lemma 2.1. Then.

$$\begin{aligned}
 M_1(\overline{G_1 + G_2}) &= |V(G_1 + G_2)|(|V(G_1 + G_2)| - 1)^2 \\
 &- 4|E(G_1 + G_2)|(|V(G_1 + G_2)| - 1) + M_1(G_1 + G_2) \\
 &= (n_1 + n_2)(n_1 + n_2 - 1)^2 - 8(m_1 + m_2 + n_1n_2)(n_1 + n_2 - 1) + M_1(G_1) \\
 &+ M_1(G_2) + n_1n_2^2 + n_2n_1^2 + 4m_1n_2 + 4m_2n_1.
 \end{aligned}$$

Theorem 3.5: Let G_1, G_2 be two graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, then

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

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

$$\begin{aligned}
 M_2(G_1 + G_2) &= \sum_{uv \in E(G_1 + G_2)} \delta_{G_1 + G_2}(u)\delta_{G_1 + G_2}(v) \\
 &= \sum_{uv \in E(G_1)} \delta_{G_1 + G_2}(u)\delta_{G_1 + G_2}(v) + \sum_{uv \in E(G_2)} \delta_{G_1 + G_2}(u)\delta_{G_1 + G_2}(v)
 \end{aligned}$$

$$\begin{aligned}
 & + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_1+G_2}(u) \delta_{G_1+G_2}(v) \\
 & = \sum_{uv \in E(G_1)} (\delta_{G_1}(u) + n_2)(\delta_{G_1}(v) + n_2) + \sum_{uv \in E(G_2)} (\delta_{G_2}(u) + n_1)(\delta_{G_2}(v) + n_1) \\
 & + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} (\delta_{G_1}(u) + n_2)(\delta_{G_2}(v) + n_1) \\
 & = \sum_{uv \in E(G_1)} [\delta_{G_1}(u) \delta_{G_1}(v) + n_2 \delta_{G_1}(u) + n_2 \delta_{G_1}(v) + n_2^2] \\
 & + \sum_{uv \in E(G_2)} [\delta_{G_2}(u) \delta_{G_2}(v) + n_1 \delta_{G_2}(u) + n_1 \delta_{G_2}(v) + n_1^2] \\
 & + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}(u) \delta_{G_2}(v) + n_1 \delta_{G_1}(u) + n_2 \delta_{G_2}(v) + n_1 n_2] \\
 & = M_2(G_1) + n_2 M_1(G_1) + n_2^2 m_1 + M_2(G_2) + n_1 M_1(G_2) + n_1^2 m_2 \\
 & + 4m_1 m_2 + 2m_1 n_1 n_2 + 2m_2 n_2 n_1 + n_1^2 n_2^2.
 \end{aligned}$$

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

$$\begin{aligned}
 M_2(\overline{G_1 + G_2}) & = \frac{1}{2} n_1 n_2 (n_1 n_2 - 1)^3 + (n_1 n_2 - \frac{3}{2}) [M_1(G_1) + M_1(G_2) + n_1 n_2^2 \\
 & + n_2 n_1^2 + 4m_1 n_2 + 4m_2 n_1] + 2[m_1 + m_2 + n_1 n_2]^2 - [M_2(G_1) + M_2(G_2) \\
 & + n_2 M_1(G_1) + n_1 M_1(G_2) + n_2^2 m_1 + n_1^2 m_2 + 4m_1 m_2 + 2m_1 n_1 n_2 \\
 & + 2m_2 n_2 n_1 + n_1^2 n_2^2] - 3(m_1 + m_2 + n_1 n_2)(n_1 n_2 - 1)^2.
 \end{aligned}$$

Proof. From Proposition 3.1. we have $M_2(\overline{G}) = \frac{1}{2} n(n-1)^3 + (n - \frac{3}{2}) M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, and since $M_1(G_1 + G_2) = M_1(G_1) + M_1(G_2) + n_1 n_2^2 + n_2 n_1^2 + 4m_1 n_2 + 4m_2 n_1$, given in Theorem 2.3. $M_2(G_1 + G_2) = M_2(G_1) + M_2(G_2) + n_2 M_1(G_1) + n_1 M_1(G_2) + n_2^2 m_1 + n_1^2 m_2 + 4m_1 m_2 + 2m_1 n_1 n_2 + 2m_2 n_2 n_1 + n_1^2 n_2^2$, given in Theorem 3.5. 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.

$$\begin{aligned}
 M_2(\overline{G_1 + G_2}) & = \frac{1}{2} |V(G_1 + G_2)| (|V(G_1 + G_2)| - 1)^3 + (|V(G_1 + G_2)| - \frac{3}{2}) M_1(G_1 + G_2) \\
 & + 2|E(G_1 + G_2)|^2 - M_2(G_1 + G_2) - 3|E(G_1 + G_2)| (|V(G_1 + G_2)| - 1)^2 \\
 & = \frac{1}{2} (n_1 + n_2)(n_1 + n_2 - 1)^3 + (n_1 + n_2 - \frac{3}{2}) [M_1(G_1) + M_1(G_2) + n_1 n_2^2 \\
 & + n_2 n_1^2 + 4m_1 n_2 + 4m_2 n_1] + 2[m_1 + m_2 + n_1 n_2]^2 - [M_2(G_1) + M_2(G_2) \\
 & + n_2 M_1(G_1) + n_1 M_1(G_2) + n_2^2 m_1 + n_1^2 m_2 + 4m_1 m_2 + 2m_1 n_1 n_2 \\
 & + 2m_2 n_2 n_1 + n_1^2 n_2^2] - 3(m_1 + m_2 + n_1 n_2)(n_1 + n_2 - 1)^2.
 \end{aligned}$$

Strong product

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

Proposition 3.7:[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

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

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

$$\begin{aligned} M_1(\overline{G_1 * G_2}) &= n_1 n_2 (n_1 n_2 - 1)^2 - 4[m_1 n_2 + n_1 m_2 + 2m_1 m_2](n_1 n_2 - 1) \\ &+ (n_2 + 6m_2)M_1(G_1) + 8m_2 m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2). \end{aligned}$$

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

$$\begin{aligned} M_1(\overline{G_1 * G_2}) &= |V(G_1 * G_2)|(|V(G_1 * G_2)| - 1)^2 \\ &- 4|E(G_1 * G_2)|(|V(G_1 * G_2)| - 1) + M_1(G_1 * G_2) \\ &= n_1 n_2 (n_1 n_2 - 1)^2 - 4[m_1 n_2 + n_1 m_2 + 2m_1 m_2](n_1 n_2 - 1) \\ &+ (n_2 + 6m_2)M_1(G_1) + 8m_2 m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2). \end{aligned}$$

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

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

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

$$\begin{aligned} M_2(G_1 * G_2) &= \sum_{(a,c)(b,d) \in E(G_1 * G_2)} [\delta_{G_1 * G_2}(a, c) + \delta_{G_1 * G_2}(b, d)] \\ &= \sum_{ab \in E(G_1)} \sum_{c=d \in V(G_2)} [(\delta_{G_1}(a) + \delta_{G_2}(c) + \delta_{G_1}(a)\delta_{G_2}(c))(\delta_{G_1}(b) + \delta_{G_2}(d) + \delta_{G_1}(b)\delta_{G_2}(d))] \\ &+ \sum_{a=b \in V(G_1)} \sum_{cd \in E(G_2)} [(\delta_{G_1}(a) + \delta_{G_2}(c) + \delta_{G_1}(a)\delta_{G_2}(c))(\delta_{G_1}(b) + \delta_{G_2}(d) + \delta_{G_1}(b)\delta_{G_2}(d))] \\ &+ \sum_{ab \in E(G_1)} \sum_{cd \in E(G_2)} [(\delta_{G_1}(a) + \delta_{G_2}(c) + \delta_{G_1}(a)\delta_{G_2}(c))(\delta_{G_1}(b) + \delta_{G_2}(d) + \delta_{G_1}(b)\delta_{G_2}(d))] \\ &= \sum_{ab \in E(G_1)} \sum_{c=d \in V(G_2)} [\delta_{G_1}(a)\delta_{G_1}(b) + \delta_{G_1}(a)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_1}(b)\delta_{G_2}(d) \\ &+ \delta_{G_2}(c)\delta_{G_1}(b) + \delta_{G_2}(c)\delta_{G_2}(d) + \delta_{G_2}(c)\delta_{G_1}(b)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_1}(b) \\ &+ \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_1}(b)\delta_{G_2}(d)] \\ &+ \sum_{a=b \in V(G_1)} \sum_{cd \in E(G_2)} [\delta_{G_1}(a)\delta_{G_1}(b) + \delta_{G_1}(a)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_1}(b)\delta_{G_2}(d) \end{aligned}$$

$$\begin{aligned}
 & + \delta_{G_2}(c)\delta_{G_1}(b) + \delta_{G_2}(c)\delta_{G_2}(d) + \delta_{G_2}(c)\delta_{G_1}(b)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_1}(b) \\
 & + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_1}(b)\delta_{G_2}(d)] \\
 & + \sum_{ab \in E(G_1)} \sum_{cd \in E(G_2)} [\delta_{G_1}(a)\delta_{G_1}(b) + \delta_{G_1}(a)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_1}(b)\delta_{G_2}(d) \\
 & + \delta_{G_2}(c)\delta_{G_1}(b) + \delta_{G_2}(c)\delta_{G_2}(d) + \delta_{G_2}(c)\delta_{G_1}(b)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_1}(b) \\
 & + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_2}(d) + \delta_{G_1}(a)\delta_{G_2}(c)\delta_{G_1}(b)\delta_{G_2}(d)] \\
 & = (n_2 + 4m_2)M_2(G_1) + 2m_2M_1(G_1) + m_1M_1(G_2) + M_1(G_2)M_1(G_1) \\
 & + M_2(G_1)M_1(G_2) + (n_1 + 4m_1)M_2(G_2) + 2m_1M_1(G_2) + m_2M_1(G_1) \\
 & + M_1(G_1)M_1(G_2) + M_2(G_2)M_1(G_1) + m_2M_2(G_1) + M_1(G_1)M_1(G_2) \\
 & + m_1M_2(G_2) + M_1(G_1)M_2(G_2) + M_1(G_2)M_2(G_1) + M_2(G_1)M_2(G_2) \\
 & = (n_2 + 5m_2)M_2(G_1) + (n_1 + 5m_1)M_2(G_2) + 3m_2M_1(G_1) + 3m_1M_1(G_2) \\
 & + 3M_1(G_1)M_1(G_2) + 2M_1(G_2)M_2(G_1) + 2M_1(G_1)M_2(G_2) + M_2(G_1)M_2(G_2).
 \end{aligned}$$

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

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

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

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

Cartesian product

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

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

$$\begin{aligned}
 M_1(\overline{G_1 \times G_2}) & = n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2 + n_1m_2)(n_1n_2 - 1) + n_2M_1(G_1) \\
 & + n_1M_1(G_2) + 8m_1m_2.
 \end{aligned}$$

Proof. From Proposition 2.2. we have $M_1(\overline{G}) = n(n-1)^2 - 4m(n-1) + M_1(G)$, and since $M_1(G_1 \times G_2) = n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2$, given in Theorem 2.4. and $|E(G_1 \times G_2)| = m_1n_2 + n_1m_2$, $|V(G_1 \times G_2)| = n_1n_2$ given in Lemma 2.1. Then.

$$\begin{aligned} M_1(\overline{G_1 \times G_2}) &= |V(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1)^2 \\ &\quad - 4|E(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1) + M_1(G_1 \times G_2) \\ &= n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2 + n_1m_2)(n_1n_2 - 1) + n_2M_1(G_1) \\ &\quad + n_1M_1(G_2) + 8m_1m_2. \end{aligned}$$

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

$$\begin{aligned} M_2(\overline{G_1 \times G_2}) &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2] \\ &\quad + 2[m_1n_2 + n_1m_2]^2 - [3m_2M_1(G_1) + 3m_1M_1(G_2) + n_1M_2(G_2) + n_2M_2(G_1)] \\ &\quad - 3(m_1n_2 + n_1m_2)(n_1n_2 - 1)^2. \end{aligned}$$

Proof. From Proposition 3.1. we have $M_2(\overline{G}) = \frac{1}{2}n(n-1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, and since $M_1(G_1 \times G_2) = n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2$, $M_2(G_1 \times G_2) = 3m_2M_1(G_1) + 3m_1M_1(G_2) + n_1M_2(G_2) + n_2M_2(G_1)$, given in Theorem 2.4. and Theorem 2.6. respectively, and $|E(G_1 \times G_2)| = m_1n_2 + n_1m_2$, $|V(G_1 \times G_2)| = n_1n_2$ given in Lemma 2.1. Then.

$$\begin{aligned} M_2(\overline{G_1 \times G_2}) &= \frac{1}{2}|V(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1)^3 + (|V(G_1 \times G_2)| - \frac{3}{2})M_1(G_1 \times G_2) \\ &\quad + 2|E(G_1 \times G_2)|^2 - M_2(G_1 \times G_2) - 3|E(G_1 \times G_2)|(|V(G_1 \times G_2)| - 1)^2 \\ &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2] \\ &\quad + 2[m_1n_2 + n_1m_2]^2 - [3m_2M_1(G_1) + 3m_1M_1(G_2) + n_1M_2(G_2) + n_2M_2(G_1)] \\ &\quad - 3(m_1n_2 + n_1m_2)(n_1n_2 - 1)^2. \end{aligned}$$

Composition

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

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

$$\begin{aligned} M_1(\overline{G_1 \circ G_2}) &= n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1)(n_1n_2 - 1) + n_2^3M_1(G_1) \\ &\quad + n_1M_1(G_2) + 8n_2m_2m_1. \end{aligned}$$

Proof. From Proposition 2.2. we have $M_1(\overline{G}) = n(n-1)^2 - 4m(n-1) + M_1(G)$, and since $M_1(G_1 \circ G_2) = n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1$, given in Theorem 2.4. 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.

$$\begin{aligned} M_1(\overline{G_1 \circ G_2}) &= |V(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1)^2 \\ &\quad - 4|E(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1) + M_1(G_1 \circ G_2) \\ &= n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1)(n_1n_2 - 1) + n_2^3M_1(G_1) \\ &\quad + n_1M_1(G_2) + 8n_2m_2m_1. \end{aligned}$$

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

$$\begin{aligned} M_2(\overline{G_1 \circ G_2}) &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1] \\ &+ 2[m_1n_2^2 + m_2n_1]^2 - [n_2^4M_2(G_1) + n_1M_2(G_2) + 3n_2^2m_2M_1(G_1) \\ &+ 2n_2m_1M_1(G_2) + 4m_1m_2^2] - 3(m_1n_2^2 + m_2n_1)(n_1n_2 - 1)^2. \end{aligned}$$

Proof. From Proposition 3.1. we have $M_2(\overline{G}) = \frac{1}{2}n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2$, and since $M_1(G_1 \circ G_2) = n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1$, $M_2(G_1 \circ G_2) = n_2^4M_2(G_1) + n_1M_2(G_2) + 3n_2^2m_2M_1(G_1) + 2n_2m_1M_1(G_2) + 4m_1m_2^2$, 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.

$$\begin{aligned} M_2(\overline{G_1 \circ G_2}) &= \frac{1}{2}|V(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1)^3 + (|V(G_1 \circ G_2)| - \frac{3}{2})M_1(G_1 \circ G_2) \\ &+ 2|E(G_1 \circ G_2)|^2 - M_2(G_1 \circ G_2) - 3|E(G_1 \circ G_2)|(|V(G_1 \circ G_2)| - 1)^2 \\ &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1] \\ &+ 2[m_1n_2^2 + m_2n_1]^2 - [n_2^4M_2(G_1) + n_1M_2(G_2) + 3n_2^2m_2M_1(G_1) \\ &+ 2n_2m_1M_1(G_2) + 4m_1m_2^2] - 3(m_1n_2^2 + m_2n_1)(n_1n_2 - 1)^2. \end{aligned}$$

Disjunction

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

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

$$\begin{aligned} M_1(\overline{G_1 \vee G_2}) &= n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1^2 - 2m_1m_2)(n_1n_2 - 1) \\ &+ (n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) \\ &+ (n_2n_1^2 - 4m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2. \end{aligned}$$

Proof. From Proposition 2.2. we have $M_1(\overline{G}) = n(n - 1)^2 - 4m(n - 1) + M_1(G)$, 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.

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

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

$$\begin{aligned} M_2(\overline{G_1 \vee G_2}) &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[(n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) \\ &+ (n_2n_1^2 - 4m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2] + 2[m_1n_2^2 + m_2n_1^2 - 2m_1m_2]^2 \\ &- [((n_1^2 - 2m_1)^2 - 2n_1^2m_1)M_2(G_2) + ((n_2^2 - 2m_2)^2 - 2n_2^2m_2)M_2(G_1) \\ &+ (2n_1^2n_2m_1 - 4m_1^2n_2)M_1(G_2) + 2n_1M_2(G_2)M_1(G_1) - 2M_2(G_2)M_2(G_1) \\ &+ 2n_2M_2(G_1)M_1(G_2) + (2n_2^2n_1m_2 - 4m_2^2n_1)M_1(G_1) - n_1n_2M_1(G_2)M_1(G_1) \\ &+ 4m_2m_1(n_2^2m_1 + n_1^2m_2)] - 3[m_1n_2^2 + m_2n_1^2 - 2m_1m_2](n_1n_2 - 1)^2. \end{aligned}$$

Proof. From Proposition 3.1.

$M_2(\overline{G}) = \frac{1}{2}n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2$, and by Theorem 2.4. and Theorem 2.6. respectively, we have

$$\begin{aligned} M_1(G_1 \vee G_2) &= (n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) + (n_2n_1^2 - 4m_1n_1)M_1(G_2) \\ &+ 8m_1m_2n_1n_2, \end{aligned}$$

$$\begin{aligned} M_2(G_1 \vee G_2) &= ((n_1^2 - 2m_1)^2 - 2n_1^2m_1)M_2(G_2) + ((n_2^2 - 2m_2)^2 - 2n_2^2m_2)M_2(G_1) \\ &+ (2n_1^2n_2m_1 - 4m_1^2n_2)M_1(G_2) + (2n_2^2n_1m_2 - 4m_2^2n_1)M_1(G_1) \\ &- n_1n_2M_1(G_2)M_1(G_1) + 2n_2M_2(G_1)M_1(G_2) + 2n_1M_2(G_2)M_1(G_1) \\ &- 2M_2(G_2)M_2(G_1) + 4m_2m_1(n_2^2m_1 + n_1^2m_2), \end{aligned}$$

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

$$\begin{aligned} M_2(\overline{G_1 \vee G_2}) &= \frac{1}{2}|V(G_1 \vee G_2)|(|V(G_1 \vee G_2)| - 1)^3 + (|V(G_1 \vee G_2)| - \frac{3}{2})M_1(G_1 \vee G_2) \\ &+ 2|E(G_1 \vee G_2)|^2 - M_2(G_1 \vee G_2) - 3|E(G_1 \vee G_2)|(|V(G_1 \vee G_2)| - 1)^2 \\ &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[(n_1n_2^2 - 4m_2n_2)M_1(G_1) + M_1(G_2)M_1(G_1) \\ &+ (n_2n_1^2 - 4m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2] + 2[m_1n_2^2 + m_2n_1^2 - 2m_1m_2]^2 \\ &- [((n_1^2 - 2m_1)^2 - 2n_1^2m_1)M_2(G_2) + ((n_2^2 - 2m_2)^2 - 2n_2^2m_2)M_2(G_1) \\ &+ (2n_1^2n_2m_1 - 4m_1^2n_2)M_1(G_2) + 2n_1M_2(G_2)M_1(G_1) - 2M_2(G_2)M_2(G_1) \\ &+ 2n_2M_2(G_1)M_1(G_2) + (2n_2^2n_1m_2 - 4m_2^2n_1)M_1(G_1) - n_1n_2M_1(G_2)M_1(G_1) \\ &+ 4m_2m_1(n_2^2m_1 + n_1^2m_2)] - 3[m_1n_2^2 + m_2n_1^2 - 2m_1m_2](n_1n_2 - 1)^2. \end{aligned}$$

Symmetric difference

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

Theorem 3.17: Let G_1, G_2 be two simple connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively, then

$$\begin{aligned} M_1(\overline{G_1 \oplus G_2}) &= n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1^2 - 4m_1m_2)(n_1n_2 - 1) \\ &+ (n_1n_2^2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) \\ &+ 8m_1m_2n_1n_2. \end{aligned}$$

Proof. From Proposition 2.2. we have $M_1(\overline{G}) = n(n-1)^2 - 4m(n-1) + M_1(G)$, 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.

$$\begin{aligned} M_1(\overline{G_1 \oplus G_2}) &= |V(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)^2 - 4|E(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1) \\ &+ M_1(G_1 \oplus G_2) \\ &= n_1n_2(n_1n_2 - 1)^2 - 4(m_1n_2^2 + m_2n_1^2 - 4m_1m_2)(n_1n_2 - 1) \\ &+ (n_1n_2^2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) \\ &+ 8m_1m_2n_1n_2. \end{aligned}$$

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

$$\begin{aligned} M_2(\overline{G_1 \oplus G_2}) &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[(n_1n_2^2 - 8m_2n_2)M_1(G_1) \\ &+ 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2] \\ &+ 2[m_1n_2^2 + m_2n_1^2 - 4m_1m_2]^2 - [(n_1^2 - 2m_1)^2 - 4n_1^2m_1]M_2(G_2) \\ &+ ((n_2^2 - 2m_2)^2 - 4n_2^2m_2)M_2(G_1) + (2n_1^2n_2m_1 - 8m_1^2n_2)M_1(G_2) \\ &+ (2n_2^2n_1m_2 - 8m_2^2n_1)M_1(G_1) - 2n_1n_2M_1(G_2)M_1(G_1) \\ &+ 8n_2M_2(G_1)M_1(G_2) + 8n_1M_2(G_2)M_1(G_1) - 16M_2(G_2)M_2(G_1) \\ &+ 4m_2m_1(n_2^2m_1 + n_1^2m_2)] - 3[m_1n_2^2 + m_2n_1^2 - 4m_1m_2](n_1n_2 - 1)^2. \end{aligned}$$

Proof. From Proposition 3.1.

$M_2(\overline{G}) = \frac{1}{2}n(n-1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, and by Theorem 2.4. and Theorem 2.6. respectively, we have

$$\begin{aligned} M_1(G_1 \oplus G_2) &= (n_1n_2^2 - 8m_2n_2)M_1(G_1) + 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) \\ &+ 8m_1m_2n_1n_2. \end{aligned}$$

$$\begin{aligned} M_2(G_1 \oplus G_2) &= ((n_1^2 - 2m_1)^2 - 4n_1^2m_1)M_2(G_2) + ((n_2^2 - 2m_2)^2 - 4n_2^2m_2)M_2(G_1) \\ &+ (2n_1^2n_2m_1 - 8m_1^2n_2)M_1(G_2) + (2n_2^2n_1m_2 - 8m_2^2n_1)M_1(G_1) \\ &- 2n_1n_2M_1(G_2)M_1(G_1) + 8n_2M_2(G_1)M_1(G_2) + 8n_1M_2(G_2)M_1(G_1) \\ &- 16M_2(G_2)M_2(G_1) + 4m_2m_1(n_2^2m_1 + n_1^2m_2). \end{aligned}$$

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.

$$\begin{aligned} M_2(\overline{G_1 \oplus G_2}) &= \frac{1}{2}|V(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)^3 + (|V(G_1 \oplus G_2)| - \frac{3}{2})M_1(G_1 \oplus G_2) \\ &+ 2|E(G_1 \oplus G_2)|^2 - M_2(G_1 \oplus G_2) - 3|E(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)^2 \\ &= \frac{1}{2}n_1n_2(n_1n_2 - 1)^3 + (n_1n_2 - \frac{3}{2})[(n_1n_2^2 - 8m_2n_2)M_1(G_1) \\ &+ 4M_1(G_1)M_1(G_2) + (n_2n_1^2 - 8m_1n_1)M_1(G_2) + 8m_1m_2n_1n_2] \\ &+ 2[m_1n_2^2 + m_2n_1^2 - 4m_1m_2]^2 - [(n_1^2 - 2m_1)^2 - 4n_1^2m_1]M_2(G_2) \\ &+ ((n_2^2 - 2m_2)^2 - 4n_2^2m_2)M_2(G_1) + (2n_1^2n_2m_1 - 8m_1^2n_2)M_1(G_2) \\ &+ (2n_2^2n_1m_2 - 8m_2^2n_1)M_1(G_1) - 2n_1n_2M_1(G_2)M_1(G_1) \\ &+ 8n_2M_2(G_1)M_1(G_2) + 8n_1M_2(G_2)M_1(G_1) - 16M_2(G_2)M_2(G_1) \\ &+ 4m_2m_1(n_2^2m_1 + n_1^2m_2)] - 3[m_1n_2^2 + m_2n_1^2 - 4m_1m_2](n_1n_2 - 1)^2. \end{aligned}$$

4 Application

In this section, first and second Zagreb index have been investigated for complement titania TiO_2 nanotubes and molecular graph of nanotorus.

Corollary 4.1: The first and second Zagreb index of complement $TiO_2[n, m]$ nanotube Fig. 1. is given by

a. $M_1(\overline{TiO_2[n, m]}) = 2n(6mn + 6n - 1)[18mn(m + 1) + 18n - 23m - 19] + 4n(19m + 12),$

b. $M_2(\overline{TiO_2[n, m]})$
 $= 3n(m + 1)(6mn + 6n - 1)^3 + 4n(6mn + 6n - \frac{3}{2})(19m + 12)$
 $+ 4n(5m + 4)[(10mn + 8n) - 3(6mn + 6n - 1)^2] - 2n(65m + 31).$

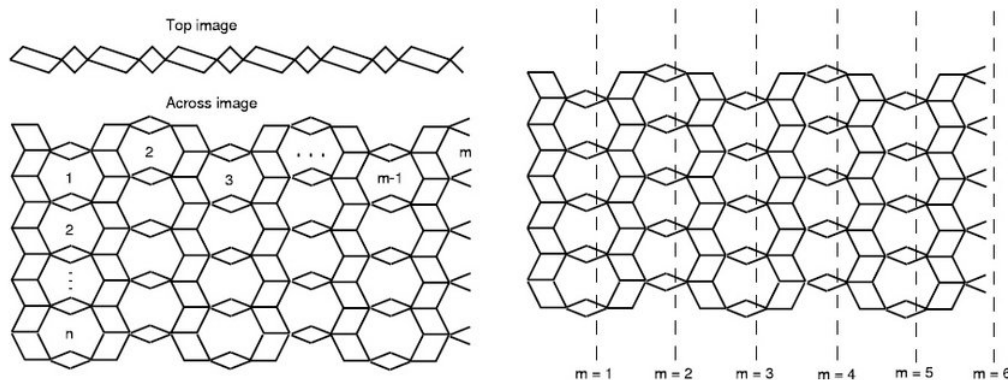


Fig. 1. The molecular graph of $TiO_2[n, m]$ nanotube

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 $M_1(TiO_2[n, m]) = 76mn + 48n$, and the partitions of the vertex set and edge set $\sum |V(TiO_2[n, m])| = 6mn + 6n$, $\sum |E(TiO_2[n, m])| = 10mn + 8n$ of titania nanotubes are given in [13, 14]. Then

$$\begin{aligned} M_1(\overline{TiO_2[n, m]}) &= \sum |V(TiO_2[n, m])|(\sum |V(TiO_2[n, m])| - 1)^2 \\ &- 4 \sum |E(TiO_2[n, m])|(\sum |V(TiO_2[n, m])| - 1) + M_1(TiO_2[n, m]) \\ &= 2n(6mn + 6n - 1)[18mn(m + 1) + 18n - 23m - 19] + 4n(19m + 12). \end{aligned}$$

Proving item(b) by Proposition 3.1 we have

$M_2(\overline{G}) = \frac{1}{2}n(n - 1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n - 1)^2$, and since $M_1(TiO_2[n, m]) = 76mn + 48n$, $M_2(TiO_2[n, m]) = 130mn + 62n$ and the partitions of the vertex set and edge set $\sum |V(TiO_2[n, m])| = 6mn + 6n$, $\sum |E(TiO_2[n, m])| = 10mn + 8n$ of titania nanotubes

are given in [14]. Hence

$$\begin{aligned}
 M_2(\overline{TiO_2[n, m]}) &= \frac{1}{2} \sum |V(TiO_2[n, m])| (\sum |V(TiO_2[n, m])| - 1)^3 \\
 &+ (\sum |V(TiO_2[n, m])| - \frac{3}{2}) M_1(TiO_2[n, m]) \\
 &+ 2[\sum |E(TiO_2[n, m])|^2 - M_2(TiO_2[n, m])] \\
 &- 3 \sum |E(TiO_2[n, m])| (\sum |V(TiO_2[n, m])| - 1)^2 \\
 &= \frac{1}{2} (6mn + 6n)(6mn + 6n - 1)^3 + (6mn + 6n - \frac{3}{2})(76mn + 48n) \\
 &+ 2[10mn + 8n]^2 - 130mn - 62n - 3(10mn + 8n)(6mn + 6n - 1)^2 \\
 &= 3n(m + 1)(6mn + 6n - 1)^3 + 4n(6mn + 6n - \frac{3}{2})(19m + 12) \\
 &+ 4n(5m + 4)[(10mn + 8n) - 3(6mn + 6n - 1)^2] - 2n(65m + 31).
 \end{aligned}$$

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. $M_1(\overline{T[p, q]}) = pq[p^2q^2 - 8pq + 16].$

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

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

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

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

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

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

$$\begin{aligned}
 M_1(\overline{P_n \times T}) &= |V(P_n \times T)|(|V(P_n \times T)| - 1)^2 - 4|E(P_n \times T)|(|V(P_n \times T)| - 1) + M_1(P_n \times T) \\
 &= npq(npq - 1)^2 - 4pq(\frac{5}{2}n - 1)(npq - 1) + pq(25n - 18) \\
 &= pq[n^3p^2q^2 - 12n^2pq + 4npq + 36n - 22].
 \end{aligned}$$

Proving item (c) by Proposition 3.1. we have $M_2(\overline{G}) = \frac{1}{2}n(n-1)^3 + (n - \frac{3}{2})M_1(G) + 2m^2 - M_2(G) - 3m(n-1)^2$, and since $M_1(T) = 9pq$, $M_2(T) = \frac{27}{2}pq$ given in [3]. Then

$$\begin{aligned} M_2(\overline{T[p, q]}) &= \frac{1}{2}|V(T)|(|V(T)| - 1)^3 + (|V(T)| - \frac{3}{2})M_1(T) + 2|E(T)|^2 - M_2(T) \\ &\quad - 3|E(T)|(|V(T)| - 1)^2 \\ &= \frac{1}{2}pq(pq - 1)^3 + 9pq(pq - \frac{3}{2}) + 2[\frac{3}{2}pq]^2 - \frac{27}{2}pq - 3\frac{3}{2}pq(pq - 1)^2 \\ &= pq[\frac{1}{2}(pq - 1)^2(pq - \frac{11}{2}) + \frac{27}{2}pq - 27]. \end{aligned}$$

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. $|E(P_n \times T)| = pq(\frac{5}{2}n - 1)$, $|V(P_n \times T)| = npq$, and by using Proposition 3.1. we get

$$\begin{aligned} M_2(\overline{P_n \times T}) &= \frac{1}{2}|V(P_n \times T)|(|V(P_n \times T)| - 1)^3 + (|V(P_n \times T)| - \frac{3}{2})M_1(P_n \times T) \\ &\quad + 2|E(P_n \times T)|^2 - M_2(P_n \times T) - 3|E(P_n \times T)|(|V(P_n \times T)| - 1)^2 \\ &= pq[\frac{1}{2}n(npq - 1)^3 + (npq - \frac{3}{2})(25n - 18) + 2pq(\frac{5}{2}n - 1)^2 \\ &\quad - \frac{1}{2}(125n - 124) - 3(\frac{5}{2}n - 1)(npq - 1)^2]. \end{aligned}$$

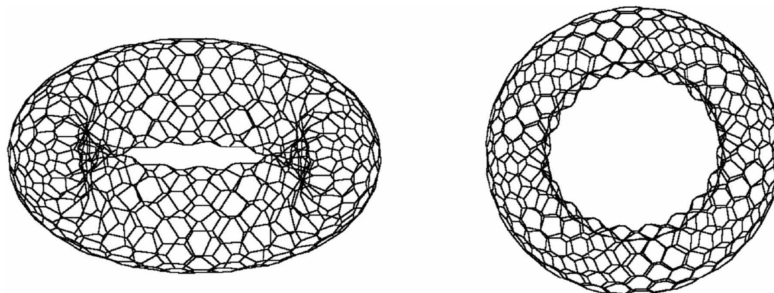


Fig. 2. Molecular graph of a nanotorus

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.

References

- [1] Li S, Zhou H. On the maximum and minimum Zagreb indices of graphs with connectivity at most k^* . Applied Mathematics Letters. 2010;23:128-132.
- [2] Gutman I, Trinajsti N. Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons. Chem. Phys. Lett. 1972;17:535-538.
- [3] Khalifeh M, Yousefi-Azari H, Ashrafi AR. The first and second Zagreb indices of some graph operations. Discrete Applied Mathematics. 2009;157(4):804-811.
- [4] Ashrafi A, Doslic T, Hamzeh A. The Zagreb coindices of graph operations. Discret. Appl.Math. 2010;158:1571-1578 .
- [5] Veylaki M, Nikmehr MJ, Tavallae HA. The third and hyper-Zagreb coindices of some graph operations. J. Appl. Math. Comput. 2016;50:315-325.
- [6] Alsharafi M, Shubatah M, Alameri A. The hyper-Zagreb index of some complement graphs. Advances in Mathematics: Scientific Journal. 2020;9(6):3631-3642.
- [7] Kiruthika K. Zagreb indices and Zagreb coindices of some graph operations. International Journal of Advanced Research in Engineering and Technology. 2016;7(3):25-41.
- [8] Alameri A, Al-Naggar N, Al-Rumaima M, Alsharafi M. Y-index of some graph operations. International Journal of Applied Engineering Research (IJAER). 2020;15(2):173-179.
- [9] Alameri A, Shubatah M, Alsharafi M. Zagreb indices, Hyper Zagreb indices and Redefined Zagreb indices of conical graph. Advances in Mathematics: Scientific Journal. 2020;9(6):3631-3642.
- [10] Ayache A, Alameri A, Ghallab A, Modabish A. Wiener polynomial and Wiener index of conical graphs. Sylwan Journal. 2020;164(3):107-116.
- [11] Behmaram A, Yousefi-Azari H, Ashrafi A. Some new results on distance-based polynomials. Commun. Math. Comput. Chem. 2011;65:39-50.
- [12] Alsharafi M, Shubatah M, Alameri A. On the Hyper-Zagreb coindex of some graphs. J. Math. Comput. Sci. 2020;10(5): 1875-1890.
- [13] Ali Malik M, Imran M. On multiple Zagreb indices of TiO_2 nanotubes. Acta Chim. Slov. 2015;62: 973-976.
- [14] De N. On molecular topological properties of TiO_2 nanotubes. Hindawi Publishing Corporation Journal of Nanoscience. 2016;5. Article ID 1028031

© 2020 Alsharafi et al.; This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>), which permits unrestricted use, distribution and reproduction in any medium, provided the original work is properly cited.

Peer-review history:

The peer review history for this paper can be accessed here (Please copy paste the total link in your browser address bar)

<http://www.sdiarticle4.com/review-history/60364>