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Computing Zagreb Connection Indices for the Cartesian Product of Path and Cycle Graphs

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ABSTRACT

Topological indices (TIs) are a class of graph-based descriptors widely used in chemiformatics and Quantitative Structure-Activity Relationship (QSAR) studies. *TIs* capture key structural features of molecules by encoding graph-theoretic information, offering a quantitative representation of molecular topology. Each mathematical network is associated with a specific numerical value determined by a TI function. Among $TIs,$ the Zagreb connection indices ($ZCIs$) have been extensively researched. This study delves into the Cartesian product of cycle graphs with path graphs, elucidating the comprehensive implications of $ZCIs$. These indices encompass the first $ZCI(FZCI)$, second $ZCI(SZCI)$, and third $ZCI(TZCI)$. Furthermore, comprehensive results of the modified first $ZCI(MFZCI)$, modified second $ZCI(MSZCI)$, and modified third $ZCI(MTZCI)$ are presented, along with the first multiplicative *ZCI* $(FMZCI),$ second multiplicative *ZCI (SMZCI),* and third multiplicative *ZCI* $(TMZCI)$. Moreover, modified first multiplicative *ZCI* $(MFMZCI)$, modified second multiplicative *ZCI* $(MSMZCI)$, and modified third multiplicative *ZCI* ($MTMZCI$) are also calculated. To provide precision, both the graphical and numerical analyses of the computed findings are aligned for the two Cartesian products.

Keywords: Cartesian product, cycle graph, path graph, topological index *(TI),* Zagreb index *(ZI),* Zagreb connection index *(ZCI)*

1. INTRODUCTION

A numerical representation is the mathematical encoding of a molecular graph that predicts the biological, structural, physicochemical, and toxicological properties of a chemical compound. These representations are also useful to investigate correlation values among various octane isomers

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[1]. Topological indices (TIs) are utilized to study the medical behavior of drugs, crystalline materials, and nanomaterials which hold significant importance in chemical and pharmaceutical industries [2]. [3–5] noted that transition indices find extensive application in researching Quantitative Structure-Activity Relationships (QSARs) and Quantitative Structure-Property Relationships (QSPRs). These relationships are crucial within the field of cheminformatics [4, 5]. The graph can be categorized into three types, namely distance, polynomial, and degree, each representing a different classification of TIs. When classification is based on distance, it is referred to as distance-based TI. Wiener initially presented distance-based TI [6] in his 1947 study on the boiling point of paraffin, which is now commonly referred to as the Wiener index. The utilization of TIs and graph invariants, derived from the distances between vertices in graphs, is prevalent in the field of mathematical chemistry [7].

Among the various classes of TIs, the degree-based class holds particular prominence, relying on vertex degrees. This category is further divided into two sub-classes, namely degree-based TIs and connection-based TIs. Gutman and Trinajstic [1] introduced these TIs to calculate the total π-electron energy of alternant hydrocarbons. These indices utilize the first Zagreb index, a well-established topological index. Additionally, Gutman and Furtula later defined two other indexes, namely the second Zagreb index (SZI) and the third Zagreb index (TZI) [8, 9]. In 2003, [10] examined a novel index known as the modified ZI. Hao [11] conducted a thorough comparison of these introduced ZIs, carefully evaluating the outcomes associated with these indices. Additionally, Das [12] delved into the investigation of various modified Zagreb indices ($MZIs$) related to graph operations.

Recently, Ali and Trinnajstic [13] introduced a novel approach to investigate the psychochemical properties of compounds. This method involves the introduction of the connection number (CN) of the vertex and the initiation of Zagreb connection indices ($ZCIs$). The number of those vertices which are at distance two from a certain vertex is said to be a CN of that vertex. They reported that the newly proposed connection-based ZIs have a better ability to forecast the psychochemical properties of various molecular structures instead of classical ZIs.
After the introduction of CN, numerous researchers embarked on investigating novel connection-based indices. Du et al. [14] applied a

connection-based modified first Zagreb index ($MFZI$) to identify extremal alkanes. In 2021, Sattar and Javaid [15] derived general expressions for calculating the modified Zagreb connection index ($MZCI$) of dendrimer nanostars. Additionally, in 2020, Ali and Javaid undertook the task of computing $MZCIs$ for T-sum graphs. Recently, Arshad et al. [16] computed the result of the Cartesian product of path and complete graphs.

Rene Descartes is credited with inventing Cartesian coordinates in the 17^{th} century, which revolutionized mathematics by establishing the first systematic connection between geometry and algebra. His analytic geometry, which gave rise to the notion, is honored by the moniker Cartesian product. The two branches of mathematics that gave rise to the concept of the Cartesian product are set theory created by Georg Cantor and analytic geometry invented by Rene Descartes. The Cartesian product of two graphs was first developed by Whitehead and Russell in 1912. Later, they were periodically /developed, most notably in 1959 by Sabidussi [17]. In 2000, Imrich et al. [18] investigated various distinct forms of network's Cartesian products. With this progression, Imrich and Peterin [19] continued to figure the *TIs* of the Cartesian products of graphs. Following the introduction of *ZCIs*, several researchers have calculated the Cartesian product of two networks attributes using $ZCIs$. Vizing [20] discovered the Cartesian product of two distinct graphs in 1963. In 2017, Shakila and Imran also investigated degree-based *TIs* for the Cartesian product of connected graphs with F-sums.

This paper presents precise solutions for connection-based fields ($ZCIs$) in the Cartesian product of path and cycle graphs. The manuscript is structured as follows. Section 2 covers elementary definitions to assist readers comprehend the core concepts. Section 3 contains the general expressions to calculate the $ZCIs$ of the Cartesian product between cycle graphs and path graphs. Finally, Section 4 presents the key findings and Section 5 states the conclusions, respectively.

2. PRELIMINARIES

This section includes key primary definitions from the literature that are essential to comprehend the main findings presented in this manuscript. **Definition 2.1.** [21] Let $\mathbb{A} = E(\mathbb{A}),\ V(\mathbb{A})$ be a graph, where $E(\mathbb{A})$ and $V(\mathbb{A})$ represent the collection of edges and vertices, respectively. Following that, the degree-based *ZIs* are defined as

1. $Z_1(\mathbb{A}) = \sum_{h\in V(\mathbb{A})} (d_{\mathbb{A}}(h))^2 = \sum_{hq\in E(\mathbb{A})} (d_{\mathbb{A}}(h) + d_{\mathrm{A}}(q)),$
2. $Z_2(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} (d_{\mathbb{A}}(h) + d_{\mathrm{A}}(q)),$

where $d_{\mathrm{A}}(h)$ and $d_{\mathrm{A}}(q)$ show the degree of the vertices h and q, respectively.

Definition 2.2. [13] For a graph $\mathbb{A}$, $FZCI$ and $SZCI$ are given as

1. $Z_1CI(\mathbb{A}) = \sum_{h\in V(\mathbb{A})} (\tau_{\mathbb{A}}(h))^2,$
2. $Z_2CI(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} (\tau_{\mathbb{A}}(h) \times \tau_{\mathbb{A}}(q)),$

where $\tau_{\mathrm{A}}(h)$ and $\tau_{\mathrm{A}}(q)$ represent the CN of the vertices h and q, respectively.

Definition 2.3. [22] For a graph $\mathbb{A}$ the $MFZCIs$, $MSZCIs$, and $MZCIs$ can be given as

1. $Z_1C^*I(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} (\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q),$
2. $Z_2C^*I(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)],$
3. $Z_3C^*I(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)].$

Definition 2.4. [23] For a graph $\mathbb{A}$, $FMZCIs$, $SMZCIs$, $TMZCIs$, and $FMZCIs$ can be defined as

1. $MZ_1CI(\mathbb{A}) = \prod_{h\in V(\mathbb{A})} \tau_{\mathbb{A}}(h)^2,$
2. $MZ_2CI(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})} (\tau_{\mathbb{A}}(h) \times \tau_{\mathbb{A}}(q)),$
3. $MZ_3CI(\mathbb{A}) = \prod_{h\in V(\mathbb{A})} (d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h)),$
4. $MZ_4CI(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})} (\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q)).$

Definition 2.5. [22] For a graph $\mathbb{A}$, $MFMZCIs$, $MSMZCIs$, and $MFMZCIs$ can be defined as

1. $MZ_1C^*I(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) \ + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)],$
2. $MZ_2C^*I(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \ + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)],$
3. $MZ_3C^*I(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \times d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)].$

3. COMBINING CYCLE GRAPHS WITH PATH GRAPHS USING CARTESIAN PRODUCT

Let $\mathbb{A}_1 \cong C_m$ be a cycle network of order m, denoted by $V(\mathbb{A}_1) = v_s: 1 \leq s \leq m$ and

$E(\mathbb{A}_1) = v_s t_s: 1 \leq s \leq m$ and $1 \leq t \leq m$ but $s \neq t$.
Now, let $\mathbb{A}_2 \cong P_n$ be a path network of order n, $V(\mathbb{A}_2) = x_s: 1 \leq s \leq n$ and

$E(\mathbb{A}_2) = x_s x_{s+1}: 1 \leq s \leq n-1$.
The Cartesian product of $\mathbb{A}_1 \times \mathbb{A}_2 \cong C_m \times \mathrm{P}_n$. The edge set, denoted by $E(\mathbb{A}_1) \times E(\mathbb{A}_2)$ is defined as follows:
(v_s, x_a) is adjacent (v_t, x_b) if

- $v_s = v_t$ and $x_a \sim x_b$,
- $x_a = x_b$ and $v_s \sim v_t$.

This section explores the Cartesian product of the cycle graph C_m with the path graph P_n, where ($m \geq 4$ and $n \geq 6$) are shown in Figure 1. Moving on to Figure 2, we delve into the structure of the Cartesian product involving the cycle graph C_4 and the path graph P_6.

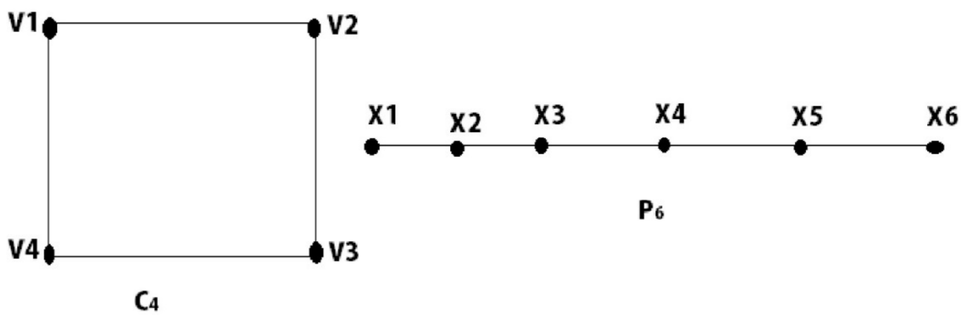

Figure 1. C_4 and P_6

At the initial level, the first layer of C_4 connects to the last edges of P_6, resulting in a CN of 3. The second layer of C_4 connects to the last layer of P_6, resulting in a CN of 4. Furthermore, the process is repeated and the 3rd, 4th, and 5th layers result in a CN of 4, although the last (6th) layer of CN is the same as the first layer. We have also labeled each edge and vertex with their degree and these CN are clearly indicated in Figure 2.

Tables 1 and 2 separately present the edge partition based on degree and CN. Tables 3 and 4 present the vertex partition based on degree and connection.

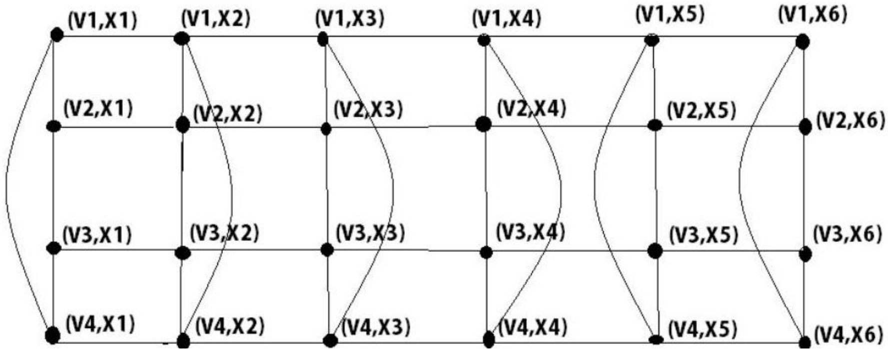

Figure 2. Cartesian Product of (C_4 and P_6)

Now, we partition the vertices and edges based on the connection and degree number of the Cartesian product with cycle graphs and path graphs.

Table 1. Degree-based Edge Partition ($C_m \times P_n$)

S.R	$E^d_{(}d(n_1), d(n_2)\big)$	Number of edges
1	$E^d_{3,3}$	$2m$
2	$E^d_{3,4}$	$2m$
3	$E^d_{4,4}$	$2mn - 5m$

Table 2. Connection-based Edge Partition ($C_m \times P_n$)

S.R	$E^c_{(}\tau(n_1), \tau(n_2)\big)$	Number of edges
1	$E^c_{4,4}$	$2m$
2	$E^c_{4,6}$	$2m$
3	$E^c_{6,6}$	$2m$
4	$E^c_{6,7}$	$2m$
5	$E^c_{7,7}$	$2mn - 9m$

Table 3. Degree-based Vertex Partition ($C_m \times P_n$)

S.R	$V^d_{(}d(n_1), d(n_2)\big)$	Number of vertices
1	V^d_3	$2m$
2	V^d_4	$m(n-2)$

Table 4. Connection-based Vertex Partition of $(C_m \times P_n)$

S.R	$V^c_{(}\tau(n_1), \tau(n_2)\big)$	Number of vertices
1	V^c_4	$2m$
2	V^c_6	$2m$
3	V^c_7	$m(n-4)$

4. RESULTS

Let $\mathbb{A} \cong C_m \times P_n$ be a graph obtained by a Cartesian product of the cycle graph (C_m) and path graph (P_n), where $m \geq 4$ and $n \geq 6$. Now, in this section we compute the main results for a graph $\mathbb{A}$.

Theorem 4.1 . For a graph $\mathbb{A}$, the $FZCI$ is given by

$FZCI\ (\mathbb{A}) = 49mn - 92m.$

Proof: Using Definition 2.2, we have

$Z_1CI(\mathbb{A}) = \sum_{h\in V(\mathbb{A})}\ [\tau_{\mathrm{A}}(h)]^2$

$= \sum_{h\in V^c_4}\ [\tau_{\mathrm{A}}(h)]^2 + \sum_{h\in V^c_6}\ [\tau_{\mathrm{A}}(h)]^2 + \sum_{h\in V^c_7}\ [\tau_{\mathrm{A}}(h)]^2$

$= |V^c_4|(4)^2 + |V^c_6|\ (6)^2 + |V^c_7|(7)^2$

$= (2m)\ (4)^2 + (2m) + m\ (n-4)\ (7)^2$

$= 49mn - 92m.$

Theorem 4.2. For a graph $\mathbb{A}$, the $SZCI$ is given by

$SZCI\ (\mathbb{A}) = 98mn - 205m.$

Proof: Using Definition 2.2, we have

$Z_2CI(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})}\ [\tau_{\mathbb{A}}(h) \times \tau_{\mathrm{A}}(q)]$

$= \sum_{hq\in E^c_{4,4}}\ [\tau_{\mathrm{A}}(h) \times \tau_{\mathrm{A}}(q)]\ + \sum_{hq\in E^c_{4,6}}\ [\tau_{\mathrm{A}}(h) \times \tau_{\mathrm{A}}(q)]$
$+ \sum_{hq\in E^c_{6,6}}\ [\tau_{\mathrm{A}}(h) \times \tau_{\mathrm{A}}(q)] + \sum_{hq\in E^c_{6,7}}\ [\tau_{\mathbb{A}}(h) \times \tau_{\mathbb{A}}(q)]$
$+ \sum_{hq\in E^c_{7,7}}\ [\tau_{\mathrm{A}}(h) \times \tau_{\mathbb{A}}(q)]$

$= \left|E^c_{4,4}\right|(4\times 4) + \left|E^c_{4,6}\right|(4\times 6) + \left|E^c_{6,6}\right|(6\times 6) + \left|E^c_{6,7}\right|(6\times 7)$
$+ \left|E^c_{7,7}\right|(7\times 7)$

$= 2m(16) + 2m(24) + 2m(36)\ + 2m(42)\ + (2mn - 9m)\ (49)$

$= 98mn - 205m.$

Theorem 4.3. For a graph $\mathbb{A}$, the $MFZCI$ is given by

$MFZCI\ (\mathbb{A}) = 28mn - 40m.$

Proof. Using Definition 2.3

$Z_1CI^*(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} [\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q)]$

$= \sum_{hq\in E^c_{4,4}} [\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q)] + \sum_{hq\in E^c_{4,6}} [\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q)] +$
$\sum_{hq\in E^c_{6,6}} [\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q)] + \sum_{hq\in E^c_{6,7}} [\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q)] +$
$\sum_{hq\in E^c_{7,7}} [\tau_{\mathbb{A}}(h) + \tau_{\mathbb{A}}(q)].$

$= |E^c_{4,4}|\ (4 + 4) + |E^c_{4,6}|\ (4 + 6) + +|E^c_{6,6}| +|E^c_{6,6}|(6 + 6) + |E^c_{6,7}|\ (6 + 7) + |E^c_{7,7}|\ (7 + 7)$

$=2m(8) + 2m(10) + 2m(13) + (2mn - 9m)(14)$

$= 28mn - 40m.$

Theorem 4.4. For a graph $\mathbb{A}$, the $MSZCI$ is given by

$MSZCI\ (\mathbb{A}) = 112mn - 188m.$

Proof: Using Definition 2.3, we have

$Z_2C^*I(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)]$

$= \sum_{hq\in\frac{E^c_{4,4}}{E^d_{3,3}}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ] + \sum_{hq\in\frac{E^c_{4,6}}{E^d_{3,4}}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ] + \sum_{hq\in\frac{E^c_{6,6}}{E^d_{4,4}}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ] + \sum_{hq\in\frac{E^c_{6,7}}{E^d_{4,4}}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ] + \sum_{hq\in\frac{E^c_{7,7}}{E^d_{4,4}}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ]$

$= \left|\frac{E^C_{4,4}}{E^d_{3,3}}\right| [\ (4 \times 3) + (4 \times 3)\ ] + \left|\frac{E^C_{4,6}}{E^d_{3,4}}\right| [\ (3 \times 6) + (4 \times 4)\ ] + \left|\frac{E^C_{6,6}}{E^d_{4,4}}\right| [\ (6 \times 4) + (6 \times 4)\ ] + \left|\frac{E^C_{6,7}}{E^d_{4,4}}\right| [\ (7 \times 4) + (4 \times 6)\ ] + \left|\frac{E^C_{7,7}}{E^d_{4,4}}\right| [\ (7 \times 4) + (7 \times 4)\ ]$

$= 2m(24) + 2m(34) + 2m(48) + 2m(52) + (2mn - 9m)(14)$

$= 112mn - 188m.$

Theorem 4.5. For a graph $\mathbb{A}$, the $MTZCI$ is given by

$MTZCI\ (\mathbb{A})\ = 112mn - 184m.$

Proof: Using Definition 2.3, we have

$Z_3C^*I(\mathbb{A}) = \sum_{hq\in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \sum_{hq\in\frac{E_{4,4}^c}{E_{3,3}^d}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] + \sum_{hq\in\frac{E_{4,6}^c}{E_{3,4}^d}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] + \sum_{hq\in\frac{E_{6,6}^c}{E_{4,4}^d}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] + \sum_{hq\in\frac{E_{6,7}^c}{E_{4,4}^d}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] + \sum_{hq\in\frac{E_{7,7}^c}{E_{4,4}^d}} [\ d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \left|\frac{E_{4,4}^c}{E_{3,3}^d}\right| [\ (4\times 3) + (4\times 3)\ ] + \left|\frac{E_{4,6}^c}{E_{3,4}^d}\right| [\ (4\times 3) + (6\times 4)\ ] + \left|\frac{E_{6,6}^c}{E_{4,4}^d}\right| [\ (6\times 4) + (6\times 4)\ ] + \left|\frac{E_{6,7}^c}{E_{4,4}^d}\right| [\ (6\times 4) + (7\times 4)\ ] + \left|\frac{E_{7,7}^c}{E_{4,4}^d}\right| [\ (7\times 4) + (7\times 4)\ ]$

$= \ 2m(24) + 2m(36) + 2m(48) + 2m(52) + (2mn - 9m)(56)$

$= 112mn - 184m.$

Theorem 4.6. For a graph $\mathbb{A}$, the $FMZCI$ is given by

$FMZCI\ (\mathbb{A}) = 112896m^3n - 451584m^3.$

Proof: Using Definition 2.4, we have

$MZ_1CI(\mathbb{A}) = \prod_{h\in V(\mathbb{A})}\ [\tau_{\mathbb{A}}(h)]^2$

$= \prod_{h\in V_4^c}\ [\tau_{\mathbb{A}}(h)]^2 \times\ \prod_{h\in V_4^c}\ [\tau_{\mathbb{A}}(h)]^2 \times\ \prod_{h\in V_4^c}\ [\tau_{\mathbb{A}}(h)]^2 \times\ \prod_{h\in V_4^c}\ [\tau_{\mathbb{A}}(h)]^2 \times \prod_{h\in V_4^c}\ [\tau_{\mathbb{A}}(h)]^2$

$= |V_4^c|(4)^2 \times |V_6^c|(6)^2 \times |V_7^c|(7)^2$

$= (2m)(4)^2 \times (2m)(6)^2 \times m(n-4)(7)^2$

$= 112896m^3n - 451584m^3.$

Theorem 4.7. For a graph $\mathbb{A}$, the $SMZCI$ is given by

$SMZCI\ (\mathbb{A}) = 9289728m^5n - 4096770084m.^5$

Proof: Using Definition 2.4, we have

$MZ_2CI(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})} [\tau_{\mathbb{A}}(h) \times \tau_{\mathrm{A}}(q)]$

$= \prod_{hq\in E^c_{4,4}} [\tau_{\mathbb{A}}(h) \times \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{4,6}} [\tau_{\mathbb{A}}(h) \times \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{6,6}} [\tau_{\mathbb{A}}(h) \times \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{6,7}} [\tau_{\mathbb{A}}(h) \times \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{7,7}} [\tau_{\mathbb{A}}(h) \times \tau_{\mathrm{A}}(q)]$.

$= |E^c_{4,4}|\,(4\times 4) \times |E^c_{4,6}|(4\times 6) \times |E^c_{6,6}|(6\times 6) \times |E^c_{6,7}|(6\times 7) \times |E^c_{7,7}|(7\times 7)$

$= 2m(16) + 2m(24) + 2m(36) + 2m(42) + (2mn - 9m)(49)$

$= 9289728m^5n - 4096770084m^5$.

Theorem 4.8. For a graph $\mathbb{A}$, the TMZCI is given by

$TMZCI\ (\mathbb{A}) = 32256m^3n - 129024m^3$.

Proof: Using Definition 2.4, we have

$MZ_3CI(\mathbb{A}) = \prod_{h\in V(\mathbb{A})} [d_{\mathbb{A}}(h)\ \tau_{\mathbb{A}}(h)\ ]$

$= \prod_{h\in\frac{E^c_4}{E^d_3}} [d_{\mathbb{A}}(h)\ \tau_{\mathbb{A}}(h)] \times \prod_{h\in\frac{E^c_6}{E^d_4}} [d_{\mathbb{A}}(h)\ \tau_{\mathbb{A}}(h)] \times \prod_{h\in\frac{E^c_7}{E^d_4}} [d_{\mathbb{A}}(h)\ \tau_{\mathbb{A}}(h)]$

$= \left|\frac{E^c_4}{E^d_3}\right| (4\times 3) \times \left|\frac{E^c_6}{E^d_4}\right| (6\times 4) \times \left|\frac{E^c_7}{E^d_4}\right| (7\times 4)$

$= 2m(12) + 2m(24) + m\ (n-4)(28)$

$= 32256m^3n - 129024m^3$.

Theorem 4.9. For a graph $\mathbb{A}$, the $FMZCI$ is given by

$FMZCI\ (\mathbb{A}) = 5591040m^5n - 25159660m^5$.

Proof: Using Definition 2.4, we have

$MZ_4CI(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})} [\tau_{\mathbb{A}}(h) + \tau_{\mathrm{A}}(q)]$

$= \prod_{hq\in E^c_{4,4}} [\tau_{\mathbb{A}}(h) + \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{4,6}} [\tau_{\mathbb{A}}(h) + \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{6,6}} [\tau_{\mathbb{A}}(h) + \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{6,7}} [\tau_{\mathbb{A}}(h) + \tau_{\mathrm{A}}(q)] \times \prod_{hq\in E^c_{7,7}} [\tau_{\mathbb{A}}(h) + \tau_{\mathrm{A}}(q)]$.

$= |E^c_{4,4}|\,(4+4) \times |E^c_{4,6}|(4+6) \times |E^c_{6,6}|(6+6) \times |E^c_{6,7}|(6+7) \times |E^c_{7,7}|(7+7)$

$= 2m(8) + 2m(10) + 2m(12) + 2m(13) + (2mn - 9m)(14)$

$= 5591040m^5n - 25159660m^5$.

Theorem 4.10. For a graph $\mathbb{A}$, the $MFMZCI$ is given by

$MFMZCI\ (\mathbb{A}) = 3449830912m^5n - 1642423910m^5$.

Proof: Using Definition 2.5, we have

$MZ_1C^*I(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ]$

$= \prod_{hq\in\frac{E^c_{4,4}}{E^d_{3,3}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ] \times \prod_{hq\in\frac{E^c_{4,6}}{E^d_{3,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ]$

$= \prod_{hq\in\frac{E^c_{6,6}}{E^d_{4,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ] \times \prod_{hq\in\frac{E^c_{6,7}}{E^d_{4,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ] \times \prod_{hq\in\frac{E^c_{6,7}}{E^d_{4,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(q) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(h)\ ]$

$= \left|\frac{E^C_{4,4}}{E^d_{3,3}}\right|[\ (4\times 3) + (4\times 3)\ ] \times \left|\frac{E^C_{4,6}}{E^d_{3,4}}\right|[\ (3\times 6) + (4\times 4)\ ] \times \left|\frac{E^C_{6,6}}{E^d_{4,4}}\right|[\ (6\times 4) + (6\times 4)] \times \left|\frac{E^C_{6,7}}{E^d_{4,4}}\right|[\ (7\times 4) + (4\times 6)\ ] \times \left|\frac{E^C_{7,7}}{E^d_{4,4}}\right|[\ (7\times 4) + (7\times 4)\ ]$

$= 2m(24) \times 2m(34) \times 2m(48) \times 2m(52) \times (2mn - 9m)(56)$

$= 3649830912m^5n - 16424239104m^5$.

Theorem 4.11. For a graph $\mathbb{A}$, the $MSMZCI$ is given by

$MSMZCI\ (\mathbb{A}) = 3649830912m^5n - 16424239104m^5$.

Proof: Using Definition 2.5, we have

$MZ_2C^*I(\mathbb{A}) = \prod_{hq\in E(\mathbb{A})}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \prod_{hq\in\frac{E^c_{4,4}}{E^d_{3,3}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] \times \prod_{hq\in\frac{E^c_{4,6}}{E^d_{3,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \prod_{hq\in\frac{E^c_{6,6}}{E^d_{4,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] \times \prod_{hq\in\frac{E^c_{6,7}}{E^d_{4,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] \times \prod_{hq\in\frac{E^c_{6,7}}{E^d_{4,4}}}[d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) + d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \left|\frac{E^C_{4,4}}{E^d_{3,3}}\right| [\ (4 \times 3) + (4 \times 3)\ ] \times \left|\frac{E^C_{4,6}}{E^d_{3,4}}\right| [\ (4 \times 3) + (6 \times 4)\ ] \times \left|\frac{E^C_{6,6}}{E^d_{4,4}}\right| [$ $(6 \times 4) + (6 \times 4)] \times \left|\frac{E^C_{6,7}}{E^d_{4,4}}\right| [\ (6 \times 4) + (7 \times 4)\ ] \times \left|\frac{E^C_{7,7}}{E^d_{4,4}}\right| [\ (7 \times 4) +$ $(7 \times 4)\ ]$

$= 2m(24) \times 2m(36) \times 2m(48) \times 2m(52) \times (2mn - 9m)(56)$

$= 3864526848m^5n - 17390370816m^5.$

Theorem 4.12. For a graph $\mathbb{A}$, the $MTMZCI$ is given by

$MTMZCI\ (\mathbb{A}) = 4.02728883 \times 10^{14}\ \mathrm{m}^5\mathrm{n} - 1.81227997 \times 10^{15}\ \mathrm{m}^5.$

Proof: Using Definition 2.5, we have

$MZ_3C^*I(\mathbb{A}) = \prod_{hq \in E(\mathbb{A})} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \times d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \prod_{hq \in \frac{E^C_{4,4}}{E^d_{3,3}}} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \times d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] \times \prod_{hq \in \frac{E^C_{4,6}}{E^d_{3,4}}} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \times$ $d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \prod_{hq \in \frac{E^C_{6,6}}{E^d_{4,4}}} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \times d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] \times \prod_{hq \in \frac{E^C_{6,7}}{E^d_{4,4}}} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \times$ $d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ] \times \prod_{hq \in \frac{E^C_{6,7}}{E^d_{4,4}}} [d_{\mathbb{A}}(h)\tau_{\mathbb{A}}(h) \times d_{\mathbb{A}}(q)\tau_{\mathbb{A}}(q)\ ]$

$= \left|\frac{E^C_{4,4}}{E^d_{3,3}}\right| [\ (4 \times 3) \times (4 \times 3)\ ] \times \left|\frac{E^C_{4,6}}{E^d_{3,4}}\right| [\ (4 \times 3) \times (6 \times 4)\ ] \times \left|\frac{E^C_{6,6}}{E^d_{4,4}}\right| [$ $(6 \times 4) \times (6 \times 4)] \times \left|\frac{E^C_{6,7}}{E^d_{4,4}}\right| [\ (6 \times 4) \times (7 \times 4)\ ] \times \left|\frac{E^C_{7,7}}{E^d_{4,4}}\right| [\ (7 \times 4) \times$ $(7 \times 4)\ ]$

$= 2m(24) \times 2m(36) \times 2m(48) \times 2m(52) \times (2mn - 9m)\ (56)$

$= 4.02728883 \times 10^{14}\ \mathrm{m}^5\mathrm{n} - 1.81227997 \times 10^{15}\ \mathrm{m}^5.$

5. COMPARATIVE ANALYSIS

In this section, we compare all the computed values of connection based *ZIs* with each other. The numerical results of the Cartesian product of path graphs with cycle graphs on the basis of connection based *ZIs* such as $FZCI$, $SZCI$, $MFZCI$, $MSZCI$, $MTZCI$, $FMZCI$, $SMZCI$, $TMZCI$, $FMZCI$, $MFMZCI$, $MSMZCI$, and $MTMZCI$ are presented in Table 5 and their graphical representation is shown in Figure 3.

Table 5. Computed Values of $FZCI$, $SZCI$, $MFZCI$, $MSZCI$, $MTZCI$, $FMZCI$, $SMZCI$, $TMZCI$, $FMZCI$, $MFMZCI$, $MSMZCI$, and $MTMZCI$ of Graph $\mathbb{A}$ for $m, n = 01,02,03, \cdots 08$

$ZCIs$	$m = 1,$ $n = 1$	$m = 2,$ $n = 2$	$m = 3,$ $n = 3$	$m = 4,$ $n = 4$	$m = 5,$ $n = 5$	$m = 6,$ $n = 6$	$m = 7,$ $n = 7$
$Z_1CI(\mathbb{A})$	40	187	432	775	1216	1755	2392
$Z_2CI(\mathbb{A})$	-107	187	677	1362	2245	1559	4597
$Z_1CI^*(\mathbb{A})$	-12	72	252	408	968	1185	1332
$Z_2C^*I(\mathbb{A})$	-76	260	820	1604	2612	3844	5300
$Z_3C^*I(\mathbb{A})$	-72	256	816	1600	2608	3840	5296
$MZ_1CI(\mathbb{A})$	-338688	-1806336	-3048192	0	14112000	48771072	116169984
$MZ_2CI(\mathbb{A})$	-4087480356	-1.3050×10^{11}	-9.8874×10^{11}	-4.1570×10^{12}	-1.1350×10^{12}	-3.3142×10^{13}	-6.7761×10^{13}
$MZ_3CI(\mathbb{A})$	-96768	-51609	-870912	-2064384	4032000	13934592	33191424
$MZ_4CI(\mathbb{A})$	-19568640	-447283200	-2037934080	-2862612480	873600000	6.5213×10^{10}	2.3492×10^{11}
$MZ_1CI^*(\mathbb{A})$	-1.6059×10^{11}	-2.9198×10^{11}	-1.6954×10^{12}	-1.8687×10^{12}	-5.1952×10^{13}	4.2571×10^{13}	1.5335×10^{14}
$MZ_2CI^*(\mathbb{A})$	-1.3525×10^{10}	-3.0916×10^{11}	-1.4086×10^{12}	1.9786×10^{12}	6.0383×10^{12}	4.5075×10^{13}	6.5335×10^{14}
$MZ_3CI^*(\mathbb{A})$	-1.4095×10^{15}	-3.2218×10^{16}	-1.4679×10^{17}	-2.0619×10^{17}	6.2926	4.6974×10^{18}	1.6921×10^{19}

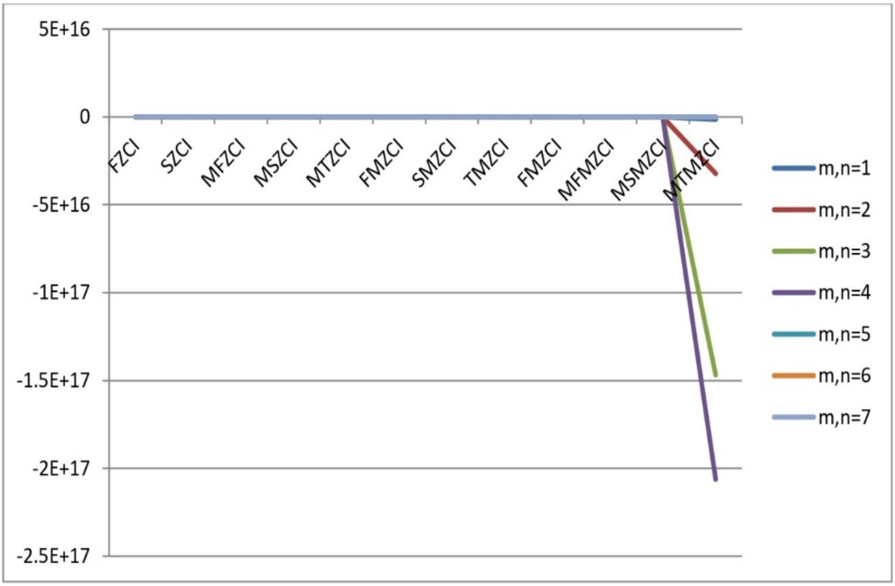

Figure 3. Computed Values of $ZCIs$ of Graph $\mathbb{A}$ for $\mathrm{m,n} = 1,2,3,\cdots 08$

By examining both Table 5 and Figure 3, it becomes evident that the Cartesian product of path graphs, cycle graphs. In Figure 3 show that $FZCI$ has consistently achieved the highest values within this network. Graphical representation in Figure 5 illustrates that $FZCI$ has a higher line than all the other $ZCIs$ within the Cartesian product of path graphs and cycle graphs. The computed results are universal and contingent solely on the values of m, n.

6. CONCLUSION

In this research, we have derived expressions to compute TIs for the Cartesian product of cycle graphs and path graphs. TIs are crucial in manipulating and analyzing chemical organizational information. The study encompasses the calculation of various *TIs*, such as the first Zagreb connection index ($FZCI$) and the second Zagreb connection index ($SZCI$). Additionally, we have computed $MFZCI$, $MSZCI$, and $MTZCI$, as well as $FMZCI$, $SMZCI$, $TMZCI$, and $FMZCI$. A comprehensive comparative analysis of all the computed *TIs* is presented, leading to the conclusion that $MFMZCI$, $MSMZCI$, and $MTMZCI$ exhibit greater efficacy in predicting the physicochemical properties of the chemical network. This mathematical investigation not only simplifies the understanding of the chosen structure but also serves as a motivation to delve into the study of organic networks. In future, we are interested to compute the *ZCIs* of other graphs, including prism graphs, line graphs etc.

DATA AVAILABILITY

The data used to support the findings of this study are included within this article. However, the reader may contact the corresponding author for more details on the data.

CONFLICT OF INTEREST

The authors of the manuscript have no financial or non-financial conflict of interest in the subject matter or materials discussed in this manuscript.

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REFERENCES

1. Gutman I, Trinajstić N. Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons. *Chem Phy Lett*. 1972;17(4):535–538. https://doi.org/10.1016/0009-2614(72)85099-1
2. Yan W, Yang BY, Yeh YN. The behavior of Wiener indices and polynomials of graphs under five graph decorations. *Appl Math Lett*. 2007;20(3):290–295. https://doi.org/10.1016/j.aml.2006.04.010
3. Todeschini R, Consonni V. *Handbook of Molecular Descriptors*. John Wiley & Sons; 2008.
4. Todeschini R, Consonni V. *Molecular Descriptors for Chemoinformatics*. John Wiley & Sons; 2009.
5. Iswarya M, Raja R, Rajchakit G, Cao J, Alzabut J, Huang C. A perspective on graph theory-based stability analysis of impulsive stochastic recurrent neural networks with time-varying delays. *Adv Diff Equ*. 2019;2019:1–21. https://doi.org/10.1186/s13662-019-2443-3
6. Wiener H. Structural determination of paraffin boiling points. *J Am Chem Soc*. 1947;69(1):17–20. https://doi.org/10.1021/ja01193a005.
7. Trinajstić N. *Chemical Graph Theory*. CRC Press; 1983.
8. Gutman I, Ruscic B, Trinajstic N, Wilson CF. Graph theory and molecular orbitals. XII. Acyclic polyenes. *J Chem Phy*. 1975;62:3399–3405. https://doi.org/10.1063/1.430994
9. Furtula B, Gutman I. A forgotten topological index. *J Math Chem*. 2015;3(4):1184–1190. https://doi.org/10.1007/s10910-015-0480-z+0

10. Zhou B, Trinajstić N. Some properties of the reformulated Zagreb indices. *J Math Chem*. 2010;48:714–719. https://doi.org/10.1007/s10910-010-9704-4
11. Hao J. Theorems about Zagreb indices and modified Zagreb indices. *Commun Math Comput Chem*. 2011;65:659–670.
12. Das KC, Yurttas A, Togan M, Cevik AS, Cangul IN. The multiplicative Zagreb indices of graph operations. *J Inequal Appl*. 2013;2013:1–4. https://doi.org/10.1186/1029-242X-2013-90
13. Ali A, Trinajstić N. A novel/old modification of the first Zagreb index. *Molecul Info*. 2018;37(6-7):e1800008. https://doi.org/10.1002/minf.201800008
14. Du Z, Ali A, Trinajstić N. Alkanes with the first three maximal/minimal modified first Zagreb connection indices. *Molecul Info*. 2019;38(4):e1800116. https://doi.org/10.1002/minf.201800116
15. Sattar A, Javaid M, Bonyah E. Connection-Based multiplicative Zagreb indices of dendrimer Nanostars. *J Math*. 2021;2021(1):e2107623. https://doi.org/10.1155/2021/2107623
16. Arshad A, Sattar A, Javaid M, Ashebo MA. Connection number-based topological indices of cartesian product of graphs. *J Math*. 2023;2023(1):e8272936. https://doi.org/10.1155/2023/8272936
17. Sabidussi G. Graph multiplication. *Math Zeitsch*. 1959;72(1):446–457. https://doi.org/10.1007/BF01162967
18. Imrich W, Klavžar S, Hammack RH. *Product Graphs: Structure and Recognition*. Wiley-Interscience; 2000.
19. Imrich W, Peterin I. Recognizing Cartesian products in linear time. *Disc Math*. 2007;307(3-5):472–483.
20. Vizing VG. The Cartesian product of graphs. *Vycisl Sistemy*. 1963;9:30–43.
21. Gutman I, Trinajstić N. Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons. *Chem Phy Lett*. 1972;17(4):535–538. https://doi.org/10.1016/0009-2614(72)85099-1
22. Javaid M, Ali U, Siddiqui K. Novel connection based Zagreb indices of several wheel-related graphs. *Comput J Combin Math*. 2021;1:1–28.
23. Ali U, Javaid M, Kashif A. Modified Zagreb connection indices of the T-sum graphs. *Main Group Metal Chem*. 2020;43(1):43–55. https://doi.org/10.1515/mgmc-2020-0005