International Journal of Maps in Mathematics
Volume 7, Issue 2, 2024, Pages:122-137
E-ISSN: 2636-7467
www.journalmim.com

ON THE HARARY INDEX OF $\Gamma(\mathbb{Z}_n)$

ARIF GÜRSOY, ALPER ÜLKER, AND NECLA KIRCALI GÜRSOY *

ABSTRACT. In this work, the Harary index of zero-divisor graphs of rings $\mathbb{Z}_n$ are calculated when n is a member of the set $\{2p, p^2, p^\lambda, pq, p^2q, pqr\}$ where p, q and r are distinct prime numbers and λ is an integer number . We give the formulas for computing the Harary index of $\Gamma(\mathbb{Z}_n)$. Moreover, the Harary index of graphs for products of rings were computed.

Keywords: Graph theory, Topological indeces, Harary index, Zero-divisor graph, Distance in graph.

2010 Mathematics Subject Classification: 05C09, 05C25, 05C12.

1. Introduction and Preliminaries

The numerical invariants of chemical graphs are used to characterize some properties of the graph of a molecule [35]. These invariants are named in the chemical literature as topological indices also known as molecular descriptors, which are a single number [21]. Topological indices have found application in various areas of chemistry, physics, mathematics, informatics, biology, etc. [1, 2, 20, 28, 29]. Topological indices have found some applications in theoretical chemistry, Chemical graph theory is a branch of mathematical chemistry that has a significant impact on the development of the chemical sciences. This study, due to its mathematical convergence, will attract many researchers.

Received:2023.11.23 *Revised:2024.01.23* *Accepted:2024.02.08*

* Corresponding author
Arif Gürsoy ⋄ arif.gursoy@ege.edu.tr; arif.gursoy@ibg.edu.tr ⋄ https://orcid.org/0000-0002-0747-9806
Alper Ülker ⋄ a.ulker@iku.edu.tr ⋄ https://orcid.org/0000-0001-5592-7450
Necla Kırcalı Gürsoy ⋄ necla.kircali.gursoy@ege.edu.tr ⋄ https://orcid.org/0000-0002-1732-9676.

Many times, nearby atoms affect each other more than distant atoms. Ivanciuc et al. defined a new molecular graph matrix for researching this interaction, namely the Harary matrix [22]. It was also called initially the reciprocal distance matrix [24]. The Harary index has been introduced independently by Plavšić et al. [31]. The Harary index is derived from the Harary matrix and has a number of exciting properties. For this reason, many researchers have studied this notion for many years [3, 10, 11, 12, 13, 14, 16, 36, 37, 38].

Graphs are a powerful tool for exploring algebraic structures, and their use has become a prominent area of research. By mapping a graph to a ring or other algebraic structures, many academics have investigated the algebraic properties of these structures using the associated graphs [4, 6, 7, 15, 17, 19, 26, 27, 30].

Let $G = (V, E)$ be a connected graph with vertex set $V(G) = \{\nu_1, \nu_2, ..., \nu_n\}$ and edge set $E(G)$ such that $|V(G)| = n$ and $|E(G)| = m$. Let $d_{i,j}$ denote by the distance between the vertices ν_i and ν_j in G. The Harary matrix of G denoted by $RD(G)$ is an $n \times n$ matrix $(RD_{i,j})$ such that [23, 31]

$$RD_{i,j} = \begin{cases} \frac{1}{d_{i,j}}, & i \neq j \\ 0, & i = j. \end{cases}$$

The Harary index of the graph G, denoted by $HI(G)$, is defined as

$$\begin{aligned} HI(G) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} RD_{i,j} \\ &= \sum_{i<j} RD_{i,j}. \end{aligned}$$

Zero-divisor graph of a commutative ring was introduced by Beck [7]. In that study, Beck constitutes a connection between graph theory and commutative ring theory. Then, Anderson and Livingston modified the definition of the zero-divisor graph of a commutative ring [4]. They defined the zero-divisor graph of a commutative ring on nonzero zero-divisor elements of the ring as follows:

Let $\mathbb{Z}_n$ be the ring of integers modulo n. The zero-divisor graph $\Gamma(\mathbb{Z}_n)$ is the simple undirected graph without loops which has its vertex set coincides with the nonzero zero-divisors of $\mathbb{Z}_n$ and two distinct vertices υ and ν in $\Gamma(\mathbb{Z}_n)$ are adjacent whenever $\upsilon\nu = 0$ in $\mathbb{Z}_n$. Zero-divisor graphs have been a topic of interest to many researchers for many years [8, 9, 32, 34].

Throughout this paper, we study Harary index of zero-divisor graphs of $\mathbb{Z}_n$ and find some formulas for computing the Harary index of $\Gamma(\mathbb{Z}_n)$ which are examined. In Section 2, we calculate Harary index of zero-divisor graphs of $\mathbb{Z}_n$ for $n \in \{2p, p^2, p^\lambda, pq, p^2q, pqr\}$ where p, q and r are distinct prime numbers and $\lambda > 2$ is an integer number. Moreover, we arrive at the Harary index of the Cartesian product of these graphs. Finally, we provide some examples to support these theorems.

2. Harary index of $\Gamma(\mathbb{Z}_n)$

Lately, the zero-divisor graph of the ring $\mathbb{Z}_n$ is popular research in spectral graph and chemical graph theory. Many researchers have examined some topological indices of zero-divisor graph of the $\mathbb{Z}_n$ [5, 17, 18, 25, 33].

Theorem 2.1. *Let $p > 2$ be a prime number, then*

$$HI(\Gamma(\mathbb{Z}_{2p})) = \frac{(p-1)(p+2)}{4}.$$

Proof. Since $\Gamma(\mathbb{Z}_{2p})$ is a star graph it is isomorphic to $K_{1,p-1}$. In this graph, the vertex set $V(\Gamma(\mathbb{Z}_{2p}))$ is divided into two distinct subsets as follow:

$$\begin{aligned} S_1 =& \{p\}, \\ S_2 =& \{2x \mid x = 1, ..., p-1\}, \end{aligned}$$

where $|S_1| = \Phi(\frac{2p}{p}) = 1$ and $|S_2| = \Phi(\frac{2p}{2}) = p-1$. $d(\upsilon, \nu) = 1$ for $\forall \upsilon \in S_1, \forall \nu \in S_2$, and $d(\upsilon, \nu) = 2$ for $\forall \upsilon, \nu \in S_2$. Therefore,

$$\begin{aligned} HI(\Gamma(\mathbb{Z}_{2p})) =& \sum_{\upsilon,\nu \in V(\Gamma(\mathbb{Z}_{2p}))} \frac{1}{d(\upsilon, \nu)} \\ =& \sum_{\upsilon \in S_1, \nu \in S_2} \frac{1}{d(\upsilon, \nu)} + \sum_{\upsilon,\nu \in S_2} \frac{1}{d(\upsilon, \nu)} \\ =& |S_2| \frac{1}{d(\upsilon, \nu)} + \frac{|S_2|(|S_2|-1)}{2} \frac{1}{d(\upsilon, \nu)} \\ =& \frac{(p-1)(p+2)}{4}. \end{aligned}$$

□

Theorem 2.2. *Let $p > 2$ be a prime number, then*

$$HI(\Gamma(\mathbb{Z}_{p^2})) = \frac{(p-1)(p-2)}{2}.$$

Proof. Since $\Gamma(\mathbb{Z}_{p^2})$ is a complete graph having $p-1$ vertices, so

$\Gamma(\mathbb{Z}_{p^2}) \cong K_{p-1}$. In a complete graph, $d(\upsilon,\nu)=1$ for $\forall \upsilon,\nu \in V(\Gamma(\mathbb{Z}_{p^2}))$. Therefore,

$$
\begin{aligned}
HI(\Gamma(\mathbb{Z}_{p^2})) &= \sum_{\upsilon,\nu \in V(\Gamma(\mathbb{Z}_{p^2}))} \frac{1}{d(\upsilon,\nu)} \\
&= \frac{(p-1)(p-2)}{2}.
\end{aligned}
$$

□

Theorem 2.3. *Let p be a prime number and $\lambda > 2$ be an integer, then*

$$HI(\Gamma(\mathbb{Z}_{p^\lambda})) = \frac{(\lambda-1)}{4}p^\lambda - \frac{(\lambda+3)}{4}p^{\lambda-1} - \frac{p^{\lfloor \frac{\lambda}{2} \rfloor}}{4} + \frac{p^{2(\lambda-1)}}{4} + 1.$$

Proof. Firstly, we suppose that λ is even.

Case 1. In the first case, there are two subpart to be considered. In the first subpart, it is considered the distance between a vertex from S_i and a vertex from S_j where $i = 2, ..., \frac{\lambda}{2}-1$ and $j = 1, 2, ..., i-1$ is 2 as $d(\upsilon,\nu) = 2$, $\upsilon \in S_i, \nu \in S_j$. So,

$$\sum_{i=2}^{\frac{\lambda}{2}-1} \sum_{j=1}^{i-1} |S_i||S_j| \frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

The next subpart is related to the distance between a vertex from S_i and a vertex from S_j where $i = \dfrac{\lambda}{2}, ..., \lambda-2$ and $j = 1, ..., \lambda-i-1$

$$\sum_{i=\frac{\lambda}{2}}^{\lambda-2} \sum_{j=1}^{\lambda-i-1} |S_i||S_j| \frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

Case 2. We consider vertex set S_i and S_j where $i = \frac{\lambda}{2}+1, ..., \lambda-1$ and $j = \lambda-1, .., i-1$. The distance between a vertex from S_i and a vertex from S_j is 1. From this,

$$\sum_{i=\frac{\lambda}{2}+1}^{\lambda-1} \sum_{j=\lambda-i}^{i-1} |S_i||S_j| \frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

Case 3. In this case, we take into account vertices in S_i where $i = 1, ..., \lambda-1$. When considering vertices $\upsilon,\nu \in S_i$ for $i \geq \frac{\lambda}{2}$, the distance is 1, otherwise 2. Hence, we get

$$\sum_{i=1}^{\frac{\lambda}{2}-1} \frac{|S_i|(|S_i|-1)}{2} \frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda}{2}}^{\lambda-1} \frac{|S_i|(|S_i|-1)}{2} \frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

Using above three cases, when λ is even, the Harary index of $\Gamma(\mathbb{Z}_{p^\lambda})$ is as follows:

$$HI(\Gamma(\mathbb{Z}_{p^\lambda})) = \sum_{i=2}^{\frac{\lambda}{2}-1}\sum_{j=1}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda}{2}}^{\lambda-2}\sum_{j=1}^{\lambda-i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda}{2}+1}^{\lambda-1}\sum_{j=\lambda-i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=1}^{\frac{\lambda}{2}-1}\frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda}{2}}^{\lambda-1}\frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)}.$$

Now, we suppose that λ is odd.

Case 1. In this case, we consider vertex sets S_i and S_j where $i = 2, ..., \frac{\lambda-1}{2}$ and $j = 1, ..., i-1$. The distance from S_i to S_j is 2 as $d(\upsilon,\nu) = 2$, where $\upsilon \in S_i$ and $\nu \in S_j$. Hence, we get

$$\sum_{i=2}^{\frac{\lambda-1}{2}}\sum_{j=i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

Also, in other part of this case, it is considered vertex sets S_i and S_j where $i = \frac{\lambda+1}{2}, ..., \lambda-2$ and $j = 1, ..., \lambda-i-1$. The distance between these vertices is also 2. So, we have

$$\sum_{i=\frac{\lambda+1}{2}}^{\lambda-2}\sum_{j=1}^{\lambda-i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

Case 2. In this case, we are interested in vertex sets S_i and S_j where $i = \frac{\lambda+1}{2}, ..., \lambda-1$ and $j = \lambda-i, ..., i-1$. The distance is $d(\upsilon,\nu) = 1$ where $\upsilon \in S_i$ and $\nu \in S_j$. Then, we have

$$\sum_{i=\frac{\lambda+1}{2}}^{\lambda-1}\sum_{j=\lambda-i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

Case 3. In this case, we are interested in vertex sets S_i and S_j where $i = \frac{\lambda+1}{2}, ..., \lambda-1$ and $j = \lambda-i, ..., i-1$. The distance is $d(\upsilon,\nu) = 1$ where $\upsilon \in S_i$ and $\nu \in S_j$. Then, we have

$$\sum_{i=\frac{\lambda+1}{2}}^{\lambda-1}\sum_{j=\lambda-i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} \qquad \upsilon \in S_i, \nu \in S_j.$$

Case 4. In the last case, it is considered vertices in S_i where $i = 1, ..., \lambda-1$. When considering vertices $\upsilon, \nu \in S_i$ for $i \geq \frac{\lambda+1}{2}$, the distance is 1, otherwise

2. So, we attain

$$\sum_{i=1}^{\frac{\lambda-1}{2}} \frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda+1}{2}}^{\lambda-1} \frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)} \qquad \upsilon\in S_i, \nu\in S_j$$

When λ is odd, using above three cases, the Harary index of $\Gamma(\mathbb{Z}_{p^\lambda})$ is as follows:

$$HI(\Gamma(\mathbb{Z}_{p^\lambda})) = \sum_{i=2}^{\frac{\lambda-1}{2}}\sum_{j=i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda+1}{2}}^{\lambda-2}\sum_{j=1}^{\lambda-i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda+1}{2}}^{\lambda-1}\sum_{j=\lambda-i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=1}^{\frac{\lambda-1}{2}}\frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)} + \sum_{i=\frac{\lambda+1}{2}}^{\lambda-1}\frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)}.$$

Therefore, Harary index of $\Gamma(\mathbb{Z}_{p^\lambda})$ in a single form is as follows:

$$HI(\Gamma(\mathbb{Z}_{p^\lambda})) = \sum_{i=2}^{\lfloor\frac{\lambda-1}{2}\rfloor}\sum_{j=i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=\lceil\frac{\lambda}{2}\rceil}^{\lambda-2}\sum_{j=1}^{\lambda-i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=\lceil\frac{\lambda+1}{2}\rceil}^{\lambda-1}\sum_{j=\lambda-i}^{i-1}|S_i||S_j|\frac{1}{d(\upsilon,\nu)} + \sum_{i=1}^{\lfloor\frac{\lambda-1}{2}\rfloor}\frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)} + \sum_{i=\lceil\frac{\lambda}{2}\rceil}^{\lambda-1}\frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)}.$$

Note that $|S_i| = \phi(\frac{\lambda}{i}) = p^{\lambda-i} - p^{\lambda-i-1}$.

$$\begin{aligned} HI(\Gamma(\mathbb{Z}_{p^\lambda})) = &\sum_{i=2}^{\lfloor\frac{\lambda-1}{2}\rfloor}\sum_{j=1}^{i}(p^{\lambda-i}-p^{\lambda-i-1})(p^{\lambda-j}-p^{\lambda-j-1})\frac{1}{2} + \\ &\sum_{i=\lceil\frac{\lambda}{2}\rceil}^{\lambda-2}\sum_{j=1}^{\lambda-i-1}(p^{\lambda-i}-p^{\lambda-i-1})(p^{\lambda-j}-p^{\lambda-j-1})\frac{1}{2} + \\ &\sum_{i=\lceil\frac{\lambda+1}{2}\rceil}^{\lambda-1}\sum_{j=\lambda-i}^{i-1}(p^{\lambda-i}-p^{\lambda-i-1})(p^{\lambda-j}-p^{\lambda-j-1}) + \\ &\sum_{i=1}^{\lfloor\frac{\lambda-1}{2}\rfloor}\frac{(p^{\lambda-i}-p^{\lambda-i-1})(p^{\lambda-i}-p^{\lambda-i-1}-1)}{2}\frac{1}{2} + \\ &\sum_{i=\lceil\frac{\lambda}{2}\rceil}^{\lambda-1}\frac{(p^{\lambda-i}-p^{\lambda-i-1})(p^{\lambda-i}-p^{\lambda-i-1}-1)}{2}. \end{aligned} \tag{2.1}$$

After reducing and simplifying Equation 2.1, we get

$$HI(\Gamma(\mathbb{Z}_{p^\lambda})) = \frac{(\lambda-1)}{4}p^\lambda - \frac{(\lambda+3)}{4}p^{\lambda-1} - \frac{p^{\lfloor \frac{\lambda}{2} \rfloor}}{4} + \frac{p^{2(\lambda-1)}}{4} + 1.$$

□

Example 2.1. *Given* $\Gamma(\mathbb{Z}_{2^7})$ *where* $p = 2$ *and* $\lambda = 7$ *as in Figure 1. We consider Harary index of* $\Gamma(\mathbb{Z}_{2^7})$ *according to Theorem 2.3 while* λ *is odd.*

$$\begin{aligned} HI(\Gamma(\mathbb{Z}_{p^\lambda})) &= \frac{(\lambda-1)}{4}p^\lambda - \frac{(\lambda+3)}{4}p^{\lambda-1} - \frac{p^{\lfloor \frac{\lambda}{2} \rfloor}}{4} + \frac{p^{2(\lambda-1)}}{4} + 1 \\ &= \frac{6}{4}2^7 - \frac{10}{4}2^6 - \frac{2^3}{4} + \frac{2^{12}}{4} + 1 \\ &= 1055. \end{aligned}$$

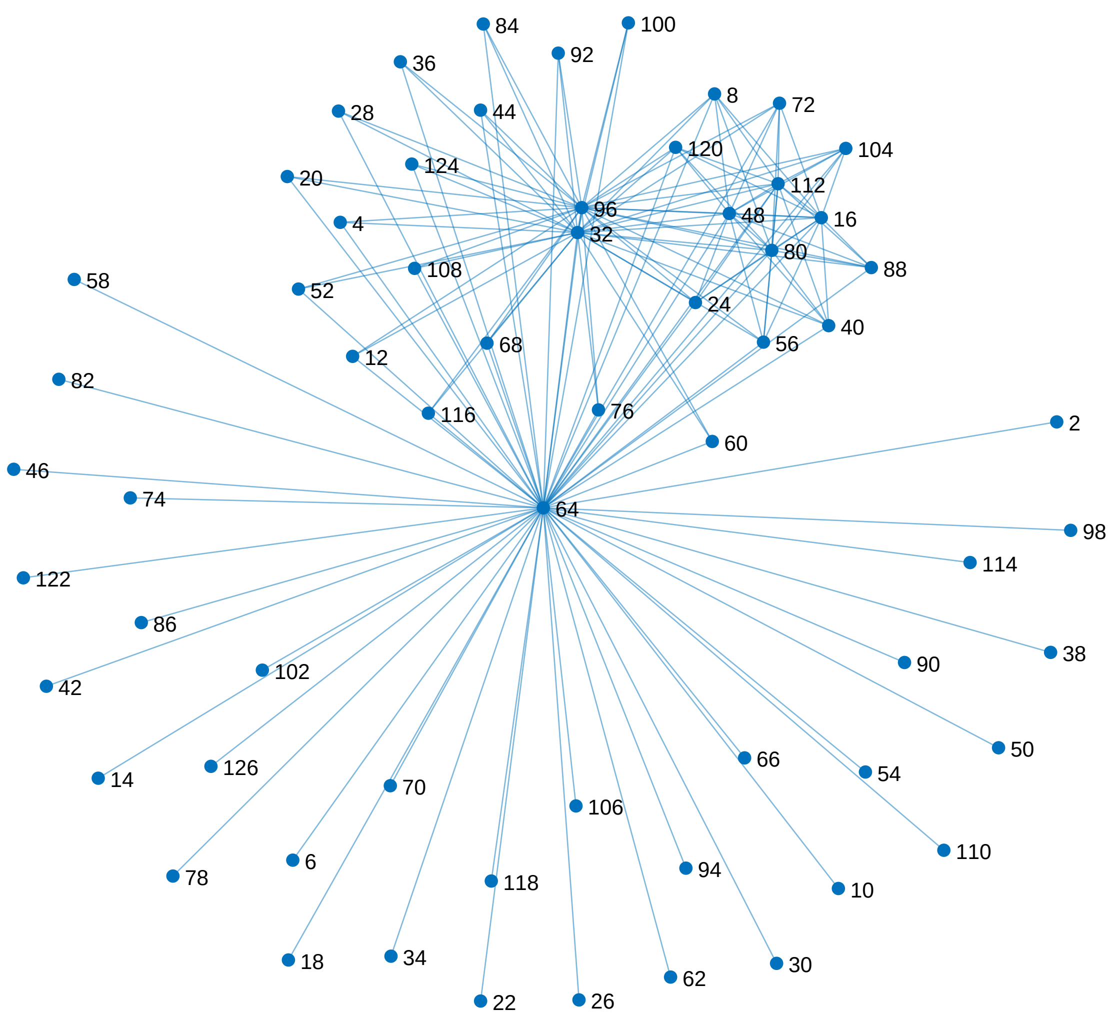

FIGURE 1. $\Gamma(\mathbb{Z}_{2^7})$

Example 2.2. *Given* $\Gamma(\mathbb{Z}_{3^6})$ *where* $p = 3$ *and* $\lambda = 6$ *as in Figure 2. In this example, we consider Harary index of* $\Gamma(\mathbb{Z}_{3^6})$ *according to Theorem 2.3 when* λ *is even.*

$$
\begin{aligned}
HI(\Gamma(\mathbb{Z}_{p^\lambda})) =& \frac{(\lambda-1)}{4}p^{\lambda} - \frac{(\lambda+3)}{4}p^{\lambda-1} - \frac{p^{\lfloor \frac{\lambda}{2} \rfloor}}{4} + \frac{p^{2(\lambda-1)}}{4} + 1 \\
=& \frac{5}{4}3^6 - \frac{9}{4}3^5 - \frac{3^3}{4} + \frac{3^{10}}{4} + 1 \\
=& 15121.
\end{aligned}
$$

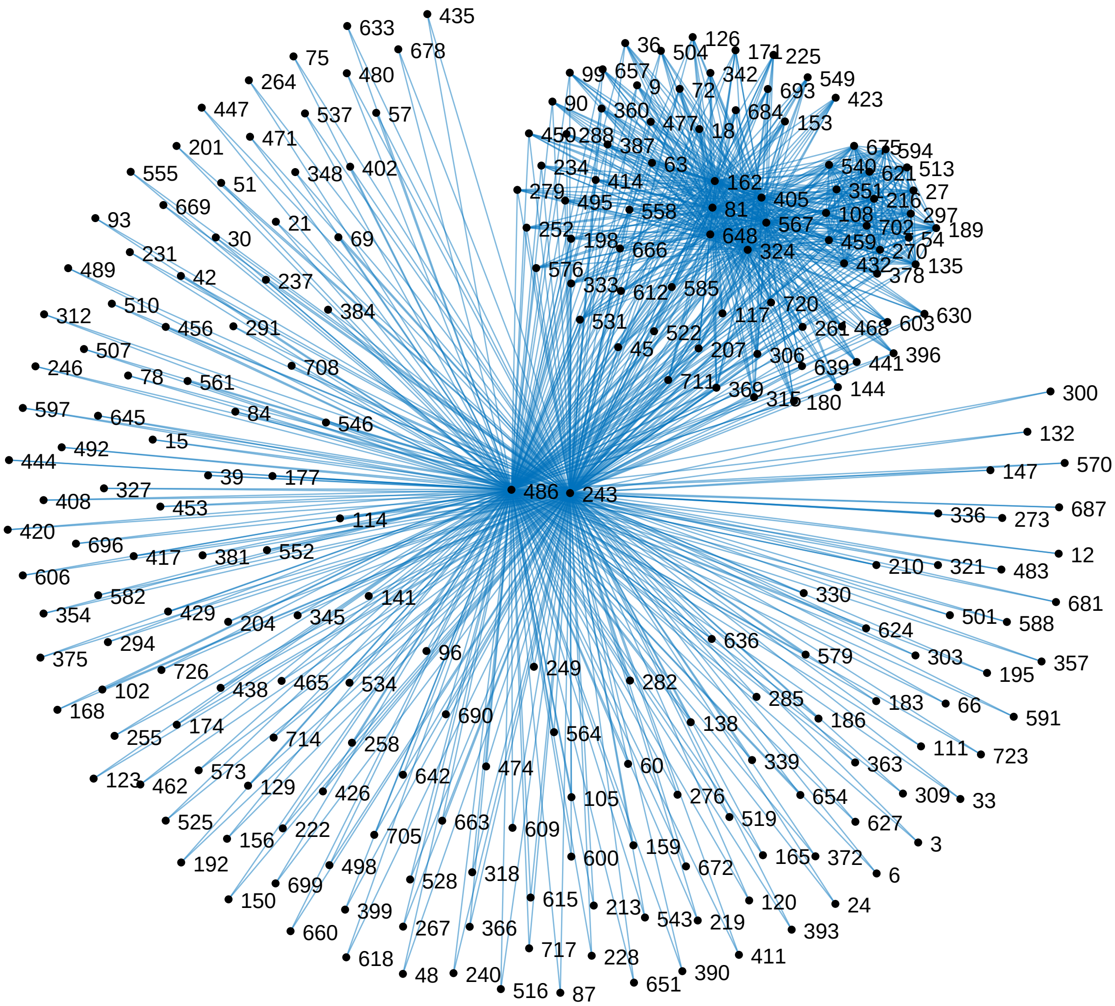

FIGURE 2. $\Gamma(\mathbb{Z}_{3^6})$

Theorem 2.4. *Let* $\Gamma(\mathbb{Z}_{pq})$ *be a zero divisor graph and* p *and* q *be distinct prime numbers, then*

$$HI(\Gamma(\mathbb{Z}_{pq})) = (p-1)(q-1)\left[1 + \frac{(p-2)}{4(q-1)} + \frac{(q-2)}{4(p-1)}\right].$$

Proof. Note that the graph $\Gamma(\mathbb{Z}_{pq})$ is isomorphic to $K_{p-1,q-1}$ which is a complete bipartite graph. The vertex set of this graph can be partitioned into two distinct subsets as

$$S_1 = \{px \mid x = 1, ..., q-1\},$$
$$S_2 = \{qx \mid x = 1, ..., p-1\},$$

where $|S_1| = \Phi(\frac{pq}{p}) = q-1$ and $|S_2| = \Phi(\frac{pq}{q}) = p-1$. It is clear that we have two cases to calculate the Harary Index.

Case 1. $d(\upsilon,\nu) = 1$ for $\forall \upsilon \in S_1$ and $\forall \nu \in S_2$ where $S_1 \cup S_2 = V(\Gamma(\mathbb{Z}_{pq}))$. Then

$$\begin{aligned}\sum_{\upsilon\in S_1,\nu\in S_2} \frac{1}{d(\upsilon,\nu)} &= |S_1|\cdot|S_2| \\ &= (p-1)(q-1).\end{aligned}$$

Case 2. $d(\upsilon,\nu) = 2$ for $\forall \upsilon,\nu \in S_i$ where $i = 1,2$. Then

$$\begin{aligned}\sum_{i=1}^{2}\sum_{\upsilon\in S_1,\nu\in S_2} \frac{1}{d(\upsilon,\nu)} &= \binom{|S_1|}{2}\cdot\frac{1}{2} + \binom{|S_2|}{2}\cdot\frac{1}{2} \\ &= \frac{1}{4}\cdot\big[(p-1)(p-2)+(q-1)(q-2)\big].\end{aligned}$$

According to these cases, we attain that

$$HI(\Gamma(\mathbb{Z}_{pq})) = (p-1)(q-1)\left[1 + \frac{(p-2)}{4(q-1)} + \frac{(q-2)}{4(p-1)}\right].$$

□

Theorem 2.5. *Let p and q be two distinct prime numbers, then Harary index of zero divisor graph $\Gamma(\mathbb{Z}_{p^2q})$ is*

$$\begin{aligned}HI(\Gamma(\mathbb{Z}_{p^2q})) = (p-1)(q-1)\bigg[&\frac{p(p+5)}{3} + \frac{(p+1)(q-1)-1}{4} \\ &+ \frac{p^3+p^2-p-4}{4(q-1)} + \frac{q-2}{4(p-1)}\bigg].\end{aligned}$$

Proof. In zero divisor graph $\Gamma(\mathbb{Z}_{p^2q})$, the vertex set is split four subsets as

$$S_1 = \{px \mid x = 1, ..., pq-1, p \nmid x, q \nmid x\},$$

$$S_2 = \{qx \mid x = 1, ..., p^2-1, p \nmid x\},$$

$$S_3 = \{p^2x \mid x = 1, ..., q-1\},$$

$$S_4 = \{pqx \mid x = 1, ..., p-1\},$$

where $\bigcup_{i=1}^{4} S_i = V(\Gamma(\mathbb{Z}_{p^2q}))$ and $S_i \cap S_j = \emptyset$ for $i, j = 1, ..., 4$, $i \neq j$.

Using these four distinct subsets, there are three possible cases to evaluate Harary index of $\Gamma(\mathbb{Z}_{p^2q})$.

Case 1. In this case, we consider (υ, ν) vertex couples where $\forall \upsilon \in S_i$ and $\forall \nu \in S_j$ for $i = 1, ..., 3$ and $j > i$. Then

$$\begin{aligned}\sum_{i=1}^{3}\sum_{j=i+1}^{4}\sum_{\upsilon\in S_i,\nu\in S_j}\frac{1}{d(\upsilon,\nu)} &= \sum_{i=1}^{3}\sum_{j=i+1}^{4}|S_i|\cdot|S_j|\cdot\frac{1}{d(\upsilon,\nu)}\Big|_{\upsilon\in S_i,\nu\in S_j}\\ &= |S_1||S_2|\frac{1}{3} + |S_1||S_3|\frac{1}{2} + |S_1||S_4|\\ &+ |S_2||S_3| + |S_2||S_4|\frac{1}{2} + |S_3||S_4|\\ &= p(p-1)(q-1)\left[2 + \frac{p-1}{3} + \frac{q-1}{2p} + \frac{p-1}{2(q-1)}\right].\end{aligned}$$

Case 2. This case takes into account two distinct vertices υ and ν where $\forall \upsilon, \nu \in S_i$ for $i = 1, ..., 3$. Then

$$\begin{aligned}\sum_{i=1}^{3}\sum_{\upsilon,\nu\in S_i}\frac{1}{d(\upsilon,\nu)} &= \sum_{i=1}^{3}|S_i|\cdot|S_i|\cdot\frac{1}{d(\upsilon,\nu)}\Big|_{\upsilon,\nu\in S_i}\\ &= \sum_{i=1}^{3}\binom{|S_i|}{2}\cdot\frac{1}{2}\\ &= \left[\binom{|S_1|}{2} + \binom{|S_2|}{2} + \binom{|S_3|}{2}\right]\cdot\frac{1}{2}\\ &= \frac{1}{4}(p-1)(q-1)\Bigg[(p-1)(q-1) - 1 + \frac{p\,(p(p-1)-1)}{q-1}\\ &\quad + \frac{q-2}{p-1}\Bigg]\end{aligned}$$

Case 3. In the last case, we consider the vertices from the S_4 which forms a complete subgraph in $\Gamma(\mathbb{Z}_{p^2q})$. Then

$$\begin{aligned}\sum_{\upsilon,\nu\in S_4}\frac{1}{d(\upsilon,\nu)} &= \frac{|S_4|(|S_4|-1)}{2} \\ &= \frac{(p-1)(p-2)}{2}.\end{aligned}$$

Evaluating above three cases, Harary index of $\Gamma(\mathbb{Z}_{p^2q})$ is

$$\begin{aligned}HI(\Gamma(\mathbb{Z}_{p^2q})) = (p-1)(q-1)\Big[&\frac{p(p+5)}{3}+\frac{(p+1)(q-1)-1}{4} \\ &+\frac{p^3+p^2-p-4}{4(q-1)}+\frac{q-2}{4(p-1)}\Big].\end{aligned}$$

□

Theorem 2.6. *Let p, q and r be three distinct prime numbers, then Harary index of zero divisor graph $\Gamma(\mathbb{Z}_{pqr})$ is*

$$\begin{aligned}HI(\Gamma(\mathbb{Z}_{pqr})) =&\alpha\beta\gamma\left(3+\frac{\alpha}{3}+\frac{\beta}{3}+\frac{\gamma}{3}\right)+\alpha\beta\left(\frac{\alpha}{2}+\frac{\beta}{2}+\frac{\alpha\beta}{4}+\frac{3}{4}\right)+ \\ &\alpha\gamma\left(\frac{\alpha}{2}+\frac{\gamma}{2}+\frac{\alpha\gamma}{4}+\frac{3}{4}\right)+\beta\gamma\left(\frac{\beta}{2}+\frac{\gamma}{2}+\frac{\beta\gamma}{4}+\frac{3}{4}\right)+ \\ &\frac{1}{4}\left(\alpha^2+\beta^2+\gamma^2-\alpha-\beta-\gamma\right)\end{aligned}$$

where $\alpha = p-1$, $\beta = q-1$, and $\gamma = r-1$.

Proof. $V(\Gamma(\mathbb{Z}_{pqr}))$ is divided into six separate subsets such as

$$S_1 = \{px \mid x = 1, ..., qr-1, q\nmid x, r\nmid x\},$$

$$S_2 = \{qx \mid x = 1, ..., pr-1, p\nmid x, r\nmid x\},$$

$$S_3 = \{rx \mid x = 1, ..., pq-1, p\nmid x, q\nmid x\},$$

$$S_4 = \{pqx \mid x = 1, ..., r-1\},$$

$$S_5 = \{prx \mid x = 1, ..., q-1\},$$

$$S_6 = \{qrx \mid x = 1, ..., p-1\}.$$

where $\bigcup_{i=1}^{6} S_i = V(\Gamma(\mathbb{Z}_{pqr}))$ and $S_i\cap S_j=\emptyset$ for $i,j=1,...,6$, $i\neq j$. Using these six distinct vertex subsets, there are three possible cases to evaluate Harary index of $\Gamma(\mathbb{Z}_{pqr})$.

Case 1. In this case, we consider (υ, ν) vertex couples where $\forall \upsilon \in S_i$ and $\forall \nu \in S_j$ for $i = 1, ..., 2$ and $j = i+1, ..., 3$, and $d(\upsilon, \nu) = 3$ according to the graph. Then

$$\begin{aligned}
\sum_{i=1}^{2}\sum_{j=i+1}^{3}\sum_{\upsilon\in S_i,\nu\in S_j}\frac{1}{d(\upsilon,\nu)} &= \sum_{i=1}^{2}\sum_{j=i+1}^{3}|S_i|\cdot|S_j|\cdot\frac{1}{d(\upsilon,\nu)}\Big|_{\upsilon\in S_i,\nu\in S_j}\\
&= |S_1||S_2|\frac{1}{3} + |S_1||S_3|\frac{1}{3} + |S_2||S_3|\frac{1}{3}\\
&= \frac{1}{3}\Big[(p-1)(q-1)(r-1)^2 + (p-1)(q-1)^2(r-1)\\
&\quad + (p-1)^2(q-1)(r-1)\Big]\\
&= \frac{(p-1)(q-1)(r-1)}{3}(p+q+r-3).
\end{aligned}$$

Case 2. This case takes into account two distinct vertex set couples S_i and S_j υ where $d(\upsilon, \nu) = 2$, $\upsilon \in S_i$ and $\nu \in S_j$. Then

$$\begin{aligned}
&\sum_{j\in\{4,5\}}\sum_{\substack{\upsilon\in S_1,\\ \nu\in S_j}}\frac{1}{d(\upsilon,\nu)} + \sum_{j\in\{4,6\}}\sum_{\substack{\upsilon\in S_2,\\ \nu\in S_j}}\frac{1}{d(\upsilon,\nu)} + \sum_{j\in\{5,6\}}\sum_{\substack{\upsilon\in S_3,\\ \nu\in S_j}}\frac{1}{d(\upsilon,\nu)}\\
&= |S_1|\cdot|S_4|\cdot\frac{1}{2} + |S_1|\cdot|S_5|\cdot\frac{1}{2} + |S_2|\cdot|S_4|\cdot\frac{1}{2} + |S_2|\cdot|S_6|\cdot\frac{1}{2}\\
&\quad + |S_3|\cdot|S_5|\cdot\frac{1}{2} + |S_3|\cdot|S_6|\cdot\frac{1}{2}\\
&= \frac{1}{2}\big[(q-1)(r-1)^2 + (q-1)^2(r-1) + (p-1)(r-1)^2 +\\
&\quad (p-1)^2(r-1) + (p-1)(q-1)^2 + (p-1)^2(q-1)\big].
\end{aligned}$$

Case 3. In this case, it is considered the vertex set couples such as S_i and S_j where $d(\upsilon, \nu) = 1$, $\upsilon \in S_i$ and $\nu \in S_j$ in $\Gamma(\mathbb{Z}_{pqr})$. Then

$$\begin{aligned}
&\sum_{i=1}^{3}\sum_{\substack{\upsilon\in S_i,\\ \nu\in S_{7-i}}}\frac{1}{d(\upsilon,\nu)} + \sum_{i=4}^{5}\sum_{j=i+1}^{6}\sum_{\substack{\upsilon\in S_i,\\ \nu\in S_j}}\frac{1}{d(\upsilon,\nu)}\\
&= |S_1|\cdot|S_6| + |S_2|\cdot|S_5| + |S_3|\cdot|S_4| + |S_4|\cdot|S_5| + |S_4|\cdot|S_6| + |S_5|\cdot|S_6|\\
&= (q-1)(r-1)(p-1) + (p-1)(r-1)(q-1) + (p-1)(q-1)(r-1) +\\
&\quad (r-1)(q-1) + (r-1)(p-1) + (q-1)(p-1).
\end{aligned}$$

Case 4. In the last case, we consider the remaining vertex couples such as $d(\upsilon,\nu)=2$ where $\upsilon,\nu\in S_i$ and $i=1,...,6$ in $\Gamma(\mathbb{Z}_{pqr})$. Then

$$\begin{aligned}\sum_{i=1}^{6}\sum_{\upsilon,\nu\in S_i}\frac{1}{d(\upsilon,\nu)}=&\sum_{i=1}^{6}\frac{|S_i|(|S_i|-1)}{2}\frac{1}{d(\upsilon,\nu)}\Big|_{\upsilon,\nu\in S_i}\\ =&\frac{1}{2}\left[\frac{(q-1)(r-1)\left[(q-1)(r-1)-1\right]}{2}\right.\\ &+\frac{(p-1)(r-1)\left[(p-1)(r-1)-1\right]}{2}\\ &+\frac{(p-1)(q-1)\left[(p-1)(q-1)-1\right]}{2}\\ &+\frac{(r-1)(r-2)}{2}\\ &\left.+\frac{(q-1)(q-2)}{2}+\frac{(p-1)(p-2)}{2}\right].\end{aligned}$$

Evaluating above all four cases, Harary index of $\Gamma(\mathbb{Z}_{pqr})$ is

$$\begin{aligned}HI(\Gamma(\mathbb{Z}_{pqr}))=&\frac{(p-1)(q-1)(r-1)}{3}(p+q+r-3)\\ &+\frac{(p-1)(q-1)(r-1)}{2}\left[\frac{r-1}{p-1}+\frac{q-1}{p-1}+\frac{r-1}{q-1}+\frac{p-1}{q-1}\right.\\ &\left.+\frac{q-1}{r-1}+\frac{p-1}{r-1}\right]\\ &+(p-1)(q-1)(r-1)\left[3+\frac{1}{p-1}+\frac{1}{q-1}+\frac{1}{r-1}\right]\\ &+\frac{(p-1)(q-1)(r-1)}{4}\left[\frac{(q-1)(r-1)-1}{p-1}+\frac{(p-1)(r-1)-1}{q-1}\right.\\ &+\frac{(p-1)(q-1)-1}{r-1}+\frac{r-2}{(p-1)(q-1)}+\frac{q-2}{(p-1)(r-1)}\\ &\left.+\frac{p-2}{(q-1)(r-1)}\right]\\ =&\alpha\beta\gamma\left(3+\frac{\alpha}{3}+\frac{\beta}{3}+\frac{\gamma}{3}\right)+\alpha\beta\left(\frac{\alpha}{2}+\frac{\beta}{2}+\frac{\alpha\beta}{4}+\frac{3}{4}\right)\\ &+\alpha\gamma\left(\frac{\alpha}{2}+\frac{\gamma}{2}+\frac{\alpha\gamma}{4}+\frac{3}{4}\right)+\beta\gamma\left(\frac{\beta}{2}+\frac{\gamma}{2}+\frac{\beta\gamma}{4}+\frac{3}{4}\right)\\ &+\frac{1}{4}\left(\alpha^2+\beta^2+\gamma^2-\alpha-\beta-\gamma\right).\end{aligned}$$

where $\alpha=p-1$, $\beta=q-1$, and $\gamma=r-1$. ☐

Theorem 2.7. *Let $\Gamma(\mathbb{Z}_p\times\mathbb{Z}_q)$, $\Gamma(\mathbb{Z}_p\times\mathbb{Z}_q\times\mathbb{Z}_r)$, $\Gamma(\mathbb{Z}_{pq})$, and $\Gamma(\mathbb{Z}_{pqr})$ be zero-divisor graphs where p, q, and r are distinct prime numbers. The followings hold:*

i) $HI(\Gamma(\mathbb{Z}_p\times\mathbb{Z}_q))=HI(\Gamma(\mathbb{Z}_{pq}))$

ii) $HI(\Gamma(\mathbb{Z}_p \times \mathbb{Z}_q \times \mathbb{Z}_r)) = HI(\Gamma(\mathbb{Z}_{pqr}))$

Proof. If $R_1 \cong R_2$, then $\Gamma(R_1) \cong \Gamma(R_2)$ [18]. Therefore proof of this theorem is clear. □

3. CONCLUSION

Topological indices is very important in chemical graph theory since they are one of these methods of studying graphs and obtaining new applications of them. We computed Harary index of the zero-divisor graphs of Zn this article. Some formulas was found for computing the Harary index of $\mathbb{Z}_n$ for $n \in \{2p, p^2, p^\lambda, pq, p^2q, pqr\}$ where p, q and r are distinct prime numbers and $\lambda > 2$ is an integer number. Finally, some examples were given support to the Theorems in this article.

References

[1] Ahmad, U., Ahmad, S., & Yousaf, R. (2017). Computation of Zagreb and atom-bond connectivity indices of certain families of dendrimers by using automorphism group action. Journal of the Serbian Chemical Society, 82(2), 151-162.

[2] Akram, M., Ahmad, U., & Rukhsar. (2022). Threshold graphs under picture Dombi fuzzy information. Granular Computing, 7(3), 691-707.

[3] Azari, M., & Iranmanesh, A. (2014). Harary index of some nano-structures. MATCH Commun. Math. Comput. Chem, 71, 373-382.

[4] Anderson, D. F., Livingston, P. S. (1999) The zero-divisor graph of a commutative ring, Journal of Algebra, 217(2), 434–447.

[5] Asir, T., & Rabikka, V. (2022). The Wiener index of the zero-divisor graph of $\mathbb{Z}_n$. Discrete Applied Mathematics, 319, 461-471.

[6] Atani, S. E., & Saraei, F. E. K. (2013). The total graph of a commutative semiring. Analele ştiinţifice ale Universităţii" Ovidius" Constanţa. Seria Matematică, 21(2), 21-33.

[7] Beck, I. (1988). Coloring of commutative rings. Journal of algebra, 116(1), 208-226.

[8] Bhat, M. I., & Pirzada, S. (2019). On strong metric dimension of zero-divisor graphs of rings. Korean Journal of Mathematics, 27(3), 563-580.

[9] Bhat, V. K., & Singh, P. (2021). ON ZERO DIVISOR GRAPH OF MATRIX RING Mn(Zp). International Journal of Applied Mathematics, 34(6), 1111.

[10] Borovićanin, B., Furtula, B., & Jerotijević, M. (2022). On the minimum Harary index of graphs with a given diameter or independence number. Discrete Applied Mathematics, 320, 331-345.

[11] Chaluvaraju, B., Boregowda, H. S., & Cangul, I. N. (2023). Generalized Harary index of certain classes of graphs. Far East Journal of Applied Mathematics, 116(1), 1-33.

[12] Cui, Z., & Liu, B. (2012). On Harary matrix, Harary index and Harary energy. MATCH Commun. Math. Comput. Chem, 68, 815-823.

[13] Das, K. C., Zhou, B., & Trinajstić, N. (2009). Bounds on Harary index. Journal of mathematical chemistry, 46, 1377-1393.

[14] Das, K. C., Xu, K., & Gutman, I. (2013). On Zagreb and Harary indices. MATCH Commun. Math. Comput. Chem, 70(1), 301-314.

[15] DeMeyer, F., & DeMeyer, L. (2005). Zero divisor graphs of semigroups. Journal of Algebra, 283(1), 190-198.

[16] Egan, M. C. G., & Antalan, J. R. M. (2022). On the Wiener and Harary Index of Splitting Graphs. European Journal of Pure and Applied Mathematics, 15(2), 602-619.

[17] Gursoy, A., Kircali Gursoy, N., Oner, T., & Senturk, I. (2021). An alternative construction of graphs by associating with algorithmic approach on MV-algebras. Soft Computing, 25(21), 13201-13212.

[18] Gürsoy, A., Ülker, A., & Gürsoy, N. K. (2022). Sombor index of zero-divisor graphs of commutative rings. Analele ştiinţifice ale Universităţii" Ovidius" Constanţa. Seria Matematică, 30(2), 231-257.

[19] Gürsoy, A. (2022). Construction of networks by associating with submanifolds of almost Hermitian manifolds. Fundamental Journal of Mathematics and Applications, 5(1), 21-31.

[20] Gursoy, A., Gursoy, N. K., & Ülker, A. (2022). Computing forgotten topological index of zero-divisor graphs of commutative rings. Turkish Journal of Mathematics, 46(5), 1845-1863.

[21] Hosoya, H. (1971). Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. Bulletin of the Chemical Society of Japan, 44(9), 2332-2339.

[22] Ivanciuc, O., Balaban, T. S., & Balaban, A. T. (1993). Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices. Journal of Mathematical Chemistry, 12(1), 309-318.

[23] Ivanciuc, O., Balaban, T. S., & Balaban, A. T. (1993). Chemical graphs with degenerate topological indices based on information on distances. Journal of mathematical chemistry, 14(1), 21-33.

[24] Janezic, D., Milicevic, A., Nikolic, S., & Trinajstic, N. (2015). Graph-theoretical matrices in chemistry. CRC Press.

[25] Kırcalı Gürsoy, N. (2021). Computing the Forgotten Topological Index for Zero Divisor Graphs of MV-Algebras. Journal of the Institute of Science and Technology, 11(4), 3072-3085. https://doi.org/10.21597/jist.944846

[26] Kırcalı Gürsoy, N., Ülker, A., & Gürsoy, A. (2022). Independent domination polynomial of zero-divisor graphs of commutative rings. Soft Computing, 26(15), 6989-6997.

[27] Kırcalı Gürsoy, N. (2023). Graphs of Wajsberg Algebras via Complement Annihilating. Symmetry, 15(1), 121.

[28] Lal, S., Kumar Bhat, V., Sharma, K., & Sharma, S. (2023). Topological indices of lead sulphide using polynomial technique. Molecular Physics, e2249131.

[29] Lal, S., Bhat, V. K., & Sharma, S. (2023). Topological indices and graph entropies for carbon nanotube Y-junctions. Journal of Mathematical Chemistry.

[30] Öztürk Sözen, E., Alsuraiheed, T., Abdioğlu, C., & Ali, S. (2023). Computing Topological Descriptors of Prime Ideal Sum Graphs of Commutative Rings. Symmetry, 15(12), 2133.

[31] Plavšić, D., Nikolić, S., Trinajstić, N., & Mihalić, Z. (1993). On the Harary index for the characterization of chemical graphs. Journal of Mathematical Chemistry, 12, 235-250.

[32] Sharma, S., & Bhat, V. K. (2022). Fault-tolerant metric dimension of zero-divisor graphs of commutative rings. AKCE International Journal of Graphs and Combinatorics, 19(1), 24-30.

[33] Singh, P., & Bhat, V. K. (2021). Adjacency matrix and Wiener index of zero divisor graph $\gamma(\mathbb{Z}_n)$. Journal of Applied Mathematics and Computing, 66, 717-732.

[34] Singh, P., & Bhat, V. K. (2022). Graph invariants of the line graph of zero divisor graph of Z n. Journal of Applied Mathematics and Computing, 68(2), 1271-1287.

[35] Trinajstic, N. (2018). Chemical graph theory. CRC press.

[36] Xu, K., Das, K. C., & Trinajstić, N. (2015). The Harary index of a graph. Heidelberg: Springer.

[37] Yu, G., & Feng, L. (2011). The Harary index of trees. arXiv preprint arXiv:1104.0920.

[38] Zhou, B., Cai, X., & Trinajstić, N. (2008). On Harary index. Journal of mathematical chemistry, 44, 611-618.

(A. Gürsoy) Department of Mathematics, Ege University, Bornova, 35040, İzmir, Türkiye

(A. Gürsoy) Izmir Biomedicine and Genome Center, Balçova, 35340, Izmir, Türkiye

(A. Ülker) Department of Mathematics and Computer Science, İstanbul Kültür University, Bakırköy, 34156 , Istanbul, Türkiye

(N. Kırcalı Gürsoy) Department of Computer Programming, Ege Vocational School, Ege University, Bornova, 35040, İzmir, Türkiye