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## ON THE TRINAJSTIC INDEX OF SOME ZERO DIVISOR GRAPHS

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**Abstract.** In this paper, the Trinajstic index, a novel topological index, is analyzed within the framework of basic concepts in Graph Theory, particularly focusing on Zero-Divisor Graphs, excluding trees. The Trinajstic index, initially developed in the context of Chemical Graph Theory, investigates chemical structures based on a distance-balance concept. After constructing a pseudocode to calculate the Trinajstic index, the relevant algorithms were implemented using MATLAB. Subsequently, MATLAB codes for generating graphs and calculating the Trinajstic index were combined to compute the index for various graphs. Formulas relating to prime-based Zero-Divisor Graphs were derived and proven.

**Keywords:** Graph theory, Chemical graph theory, Topological index, Trinajstic index, Zero-divisor graphs

**2020 Mathematics Subject Classification:** 05C09, 05C25.

### 1. INTRODUCTION

Graph theory plays a crucial role in many areas of science. Nowadays, graph theory is particularly essential in chemistry for representing chemical molecules as graphs, enabling deeper analysis and a better understanding of their structures. This necessitated the development of chemical graph theory. In chemical graph theory, numerous topological indices have emerged, including the Wiener index, Szeged index, Harary index, and others. Some topological indices are computed using the degrees of a graph, while others are determined based on the distances between its vertices. Additionally, various features can be explored to understand how different topological indices are calculated and what aspects they are related to. In 2022, the Trinajstic index, which will briefly be referred to as *NT*, was introduced by Boris Furtula [11]. He provided information on this index in the context of complete graphs, cycle graphs, path graphs, star graphs, and trees. This topological index is based on distances between vertices to determine whether the structure is balanced. It is particularly relevant in chemical graph theory for understanding the balance of chemical structures.

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## 2. PRELIMINARIES

The zero divisor graph is distinct from other types of graphs because of its construction. Zero divisor graph was studied on by I. Beck [4] and its construction is related to commutative rings that is related to algebraic combinatorics. Beck's definition for the zero divisor graph is that graph consists of vertices in  $R$ . If any two vertices of graph yields  $xy = 0$ , graph is zero divisor graph.

The Trinajstic index was defined for connected, undirected and simple graph  $G$  as follows:

$$NT(G) = \sum_{u,v \in V(G)} (n_u - n_v)^2 \quad (2.1)$$

where  $n_u$  is number of vertices closer to  $u$  than  $v$ ,  $n_v$  is number of vertices closer to  $v$  than  $u$ .

This topological index is distance-based, and can also be referred to as distance-balance-based topological index to understand of graph structure.

### 3. TRINAJSTIC TOPOLOGICAL INDEX OF $\Gamma(\mathbb{Z}_n)$

Zero divisor graph of  $\mathbb{Z}$  is popular for especially in chemical graph theory. For that reason the Trinajstic index could be also considered on zero divisor graphs for  $n = \rho^2$ ,  $n = \rho^3$ ,  $n = pq$ ,  $n = \rho^2q$  and  $n = pqr$ . In this section, we will focus on Trinajstic index of  $\Gamma(\mathbb{Z}_n)$ .

**Theorem 3.1.** *Let  $\rho$  be a prime number and be  $n = \rho^3$ . Trinajstic index of  $\Gamma(\mathbb{Z}_{\rho^3})$  is as follows:*

$$NT(\Gamma(\mathbb{Z}_{\rho^3})) = \rho(\rho^2 - \rho - 1)^2(\rho - 1)^2. \quad (3.2)$$

*Proof.* Vertex set of zero divisor graph could be partitioned as  $V(\Gamma(\mathbb{Z}_{\rho^3})) = V_1 \cup V_2$  and for  $i, j \in 1, 2$  there are two subsets of  $(\Gamma(\mathbb{Z}_{\rho^3}))$  such that

$$V_1 = \{\rho\alpha \mid \alpha = 1, 2, \dots, \rho^2 - 1, \rho \nmid \alpha\},$$

$$V_2 = \{\rho^2\alpha \mid \alpha = 1, 2, \dots, \rho - 1\} \text{ where } V_1 \cap V_2 = \emptyset.$$

In addition property of zero divisor graph with  $n = \rho^3$ ,  $|V_1| = \rho(\rho - 1)$  and  $|V_2| = \rho - 1$  for all  $u \in V_1$  and  $v \in V_2$ ,  $n_u$  and  $n_v$  as follow:

$$n_u = |V_2| \text{ and}$$

$$n_v = 1. \text{ Then,}$$

$$\begin{aligned} NT(\Gamma(\mathbb{Z}_{\rho^3})) &= \sum_{\{u,v\} \in V(\Gamma(\mathbb{Z}_{\rho^3}))} (n_u - n_v)^2 \\ &= |V_1| |V_2| (|V_1| - 1)^2 \\ &= \rho(\rho^2 - \rho - 1)^2(\rho - 1)^2. \end{aligned}$$

□

The results for  $\Gamma(\mathbb{Z}_{\rho^3})$  for prime  $\rho < 20$  are listed in Table 3.1.

TABLE 3.1. Results of  $\Gamma(\mathbb{Z}_{\rho^3})$ 

$\rho$	$n = \rho^3$	NT
2	8	2
3	27	300
5	125	28880
7	343	423612
11	1331	13069100
13	2197	44974800
17	4913	319615232
19	6859	715825836

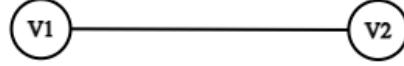
**Theorem 3.2.** Let  $\rho$  and  $q$  be prime numbers and  $n = \rho q$ . Trinajstic index of  $\Gamma(\mathbb{Z}_{\rho q})$  is as follows:

$$NT(\Gamma(\mathbb{Z}_{\rho q})) = (\rho - 1)(q - 1)(\rho - q)^2 \quad (3.3)$$

*Proof.* Vertex set of zero divisor graph could be partitioned as  $V(\Gamma(\mathbb{Z}_{\rho q})) = V_1 \cup V_2$  and for  $i, j \in 1, 2$  there are two subsets of  $(\Gamma(\mathbb{Z}_{\rho q}))$  such that

$$\begin{aligned} V_1 &= \{\rho\alpha \mid \alpha = 1, 2, \dots, q - 1\}, \\ V_2 &= \{q\alpha \mid \alpha = 1, 2, \dots, \rho - 1\} \text{ where } V_1 \cap V_2 = \emptyset. \end{aligned}$$

Since  $|V_1| = q - 1$  and  $|V_2| = \rho - 1$ ,  $\Gamma(\mathbb{Z}_{\rho q})$  has  $(\rho - 1)(q - 1)$  vertices. For set of sets pair  $V_1, V_2$ , we are able to construct graph as follow:

FIGURE 1. Structure of  $\Gamma(\mathbb{Z}_{\rho q})$ 

for all  $u \in V_1$  and  $v \in V_2$ ,  $n_u$  and  $n_v$  are as follow:  $n_u = |V_1|$  and  $n_v = |V_2|$ . Therefore  $(n_u - n_v)^2 = (|V_1| - |V_2|)^2$ . Now, we can calculate NT as

$$\begin{aligned} NT(\Gamma(\mathbb{Z}_{\rho q})) &= \sum_{\{u,v\} \in V(\Gamma(\mathbb{Z}_{\rho q}))} (n_u - n_v)^2 \\ &= |V_1| |V_2| (|V_2| - |V_1|)^2 \\ &= (\rho - 1)(q - 1)(\rho - q)^2. \end{aligned}$$

□

Results pertaining to  $\Gamma(\mathbb{Z}_{\rho q})$  for primes  $\rho < 50$  and  $q < 50$  are summarized in Table 5.2.

**Theorem 3.3.** Let  $\rho$  and  $q$  be distinct prime numbers and  $n = \rho^2 q$ . Trinajstic index of  $\Gamma(\mathbb{Z}_{\rho^2 q})$  is as follows:

$$\begin{aligned} NT(\Gamma(\mathbb{Z}_{\rho^2 q})) &= \rho(\rho - 1)(\rho^5 q - \rho^5 - 2\rho^4 q^2 + \rho^4 q + \rho^4 + \rho^3 q^3 + 13\rho^3 q^2 - 19\rho^3 q + \\ &\quad 6\rho^3 - 3\rho^2 q^3 - 24\rho^2 q^2 + 36\rho^2 q - 14\rho^2 + 4\rho q^3 + 6\rho q^2 - 3\rho q + \rho - q^2 - 5q + 2) \end{aligned} \quad (3.4)$$

*Proof.* Since  $\rho$ ,  $\rho^2$  and  $q$  are divisors of  $n = \rho^2q$ , Vertex set of zero divisor graph could be partitioned as  $V(\Gamma(\mathbb{Z}_n)) = V_1 \cup V_2 \cup V_3 \cup V_4$ ,  $i \neq j$  and for  $i, j \in 1, \dots, 4$  there are four subsets of  $(\Gamma(\mathbb{Z}_{\rho^2q}))$  such that

$$V_1 = \{\rho\alpha \mid \alpha = 1, 2, \dots, \rho q - 1, \rho \nmid \alpha, q \nmid \alpha\},$$

$$V_2 = \{q\alpha \mid \alpha = 1, 2, \dots, \rho^2 - 1, \rho \nmid \alpha\},$$

$$V_3 = \{\rho^2\alpha \mid \alpha = 1, 2, \dots, q - 1\} \text{ and}$$

$$V_4 = \{\rho q\alpha \mid \alpha = 1, 2, \dots, \rho - 1\}.$$

Size of each subsets are  $|V_1| = (\rho - 1)(q - 1)$ ,  $|V_2| = \rho(\rho - 1)$ ,  $|V_3| = (q - 1)$ ,  $|V_4| = (\rho - 1)$ , respectively. Graph was constructed by using  $V_1$ ,  $V_2$ ,  $V_3$  and  $V_4$  is below:

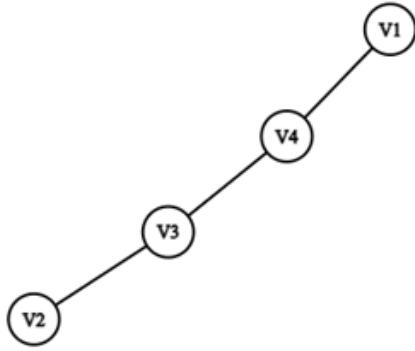


FIGURE 2. Structure of  $\Gamma(\mathbb{Z}_{\rho^2q})$

In order to calculate Trinajstic index of  $\Gamma(\mathbb{Z}_{\rho^2q})$  we must investigate these cases below:

**Case 1:** For the pair of sets  $V_1$  and  $V_2$  with  $u \in V_1$  and  $v \in V_2$ ,  $n_u$  and  $n_v$  are determined as follows:

$$n_u = |V_4| + |V_1|,$$

$$n_v = |V_3| + |V_2|.$$

$$\text{Thus, } (n_u - n_v)^2 = (|V_4| + |V_1| - (|V_3| + |V_2|))^2.$$

**Case 2:** For the pair of sets  $V_1$  and  $V_3$  with  $u \in V_1$  and  $v \in V_3$ ,  $n_u$  and  $n_v$  are as follows:

$$n_u = 1,$$

$$n_v = |V_2| + 1.$$

$$\text{Hence, } (n_u - n_v)^2 = (1 - |V_2| + 1)^2 = |V_2|^2.$$

**Case 3:** For the pair of sets  $V_1$  and  $V_4$  with  $u \in V_1$  and  $v \in V_4$ ,  $n_u$  and  $n_v$  are described as follows:

$$n_u = 1,$$

$$n_v = |V_1| + |V_2| + |V_3|.$$

$$\text{Thus, } (n_u - n_v)^2 = (|V_1| + |V_2| + |V_3| - 1)^2.$$

**Case 4:** For the pair of sets  $V_2$  and  $V_3$  with  $u \in V_2$  and  $v \in V_3$ ,  $n_u$  and  $n_v$  values can be expressed as follows::

$$n_u = |V_3|,$$

$$n_v = |V_1| + |V_2| + |V_4|.$$

Therefore,  $(n_u - n_v)^2 = (|V_1| + |V_2| + |V_4| - |V_3|)^2$ .

**Case 5:** For the pair of sets  $V_2$  and  $V_4$  with  $u \in V_2$  and  $v \in V_4$ ,  $n_u$  and  $n_v$  are as follows:

$$n_u = 1,$$

$$n_v = |V_1| + |V_4|.$$

$$\text{Hence, } (n_u - n_v)^2 = (|V_1| + |V_4| - 1)^2.$$

**Case 6:** For the pair of sets  $V_3$  and  $V_4$  with  $u \in V_3$  and  $v \in V_4$ ,  $n_u$  and  $n_v$  are described as follows:

$$n_u = 1 + |V_2|,$$

$$n_v = |V_1| + |V_3| + 1 - 1 = |V_1| + |V_3|.$$

$$\text{Thus, } (n_u - n_v)^2 = (|V_1| + |V_4| - 1)^2.$$

In this way, Trinajstic index of  $\Gamma(\mathbb{Z}_{(\rho^2 q)})$  is

$$\begin{aligned} NT(\Gamma(\mathbb{Z}_{\rho^2 q})) &= \sum_{\{u,v\} \in V(\Gamma(\mathbb{Z}_{\rho^2 q}))} (n_u - n_v)^2 \\ &= |V_1||V_3||V_2|^2 + |V_1||V_4|(|V_1| + |V_2| + |V_3| - 1)^2 + \\ &\quad |V_2||V_3|(|V_1| + |V_2| + |V_4| - |V_3|)^2 + \\ &\quad |V_2||V_4|(|V_1| + |V_4| - 1)^2 + |V_3||V_4|(|V_1| + |V_4| - 1)^2 \end{aligned}$$

Then this equation will be

$$\begin{aligned} NT(\Gamma(\mathbb{Z}_{\rho^2 q})) &= \rho(\rho - 1)(\rho^5q - \rho^5 - 2\rho^4q^2 + \rho^4q + \rho^4 + \rho^3q^3 + 13\rho^3q^2 - 19\rho^3q + 6\rho^3 - \\ &\quad 3\rho^2q^3 - 24\rho^2q^2 + 36\rho^2q - 14\rho^2 + 4\rho q^3 + 6\rho q^2 - 3\rho q + \rho - q^2 - 5q + 2). \end{aligned}$$

□

Table 5.3 provides the results for  $\Gamma(\mathbb{Z}_{\rho^2 q})$  for primes  $\rho < 20$  and  $q < 20$ .

**Theorem 3.4.** Let  $\rho$ ,  $q$  and  $r$  be distinct prime numbers and  $n = \rhoqr$ . Trinajstic index of  $\Gamma(\mathbb{Z}_{\rhoqr})$  is as follows:

$$\begin{aligned} NT(\Gamma(\mathbb{Z}_{\rhoqr})) &= (\rho - 1)^2(r - 1)(\rho q - 2q - \rho + qr + 1)^2 + \\ &\quad (q - 1)^2(r - 1)(\rho q - q - 2\rho + \rho r + 1)^2 + \\ &\quad (\rho - 1)^2(q - 1)(\rho r - 2r - \rho + qr + 1)^2 + \\ &\quad (q - 1)(r - 1)^2(\rho q - r - 2\rho + \rho r + 1)^2 + \\ &\quad (\rho - 1)(q - 1)^2(\rho r - 2r - q + qr + 1)^2 + \\ &\quad (\rho - 1)(r - 1)^2(\rho q - r - 2q + qr + 1)^2 + \\ &\quad (\rho - 1)(q - 1)(r - 1)(\rho q - q - 3r - \rho + \rho r + qr + 2)^2 + \\ &\quad (\rho - 1)(q - 1)(r - 1)(\rho q - 3q - r - \rho + \rho r + qr + 2)^2 + \\ &\quad (\rho - 1)(q - 1)(r - 1)(\rho q - q - r - 3\rho + \rho r + qr + 2)^2 + \\ &\quad r^2(\rho - q)^2(\rho - 1)(q - 1) + q^2(\rho - r)^2(\rho - 1)(r - 1) + \\ &\quad \rho^2(q - r)^2(q - 1)(r - 1) + (\rho - r)^2(\rho - 1)(q - 1)^2(q - 2)^2(r - 1) + \\ &\quad (q - r)^2(\rho - 1)^2(\rho - 2)^2(q - 1)(r - 1) + \\ &\quad (\rho - q)^2(\rho - 1)(q - 1)(r - 1)^2(r - 2)^2. \end{aligned}$$

*Proof.* Since  $\rho$ ,  $q$ ,  $r$ ,  $\rho q$ ,  $\rho r$  and  $qr$  are divisors of  $n = \rho qr$ , vertex set of zero divisor graph could be partitioned as  $V(\Gamma(\mathbb{Z}_n)) = V_1 \cup V_2 \cup V_3 \cup V_4 \cup V_5 \cup V_6$ ,  $i \neq j$  and for  $i, j \in 1, 2, \dots, 6$ . There are six subsets of  $V(\Gamma(\mathbb{Z}_{\rho qr}))$  such that

$$\begin{aligned}V_1 &= \{\rho\alpha | \alpha = 1, 2, \dots, qr - 1, q \nmid \alpha, r \nmid \alpha\}, \\V_2 &= \{q\alpha | \alpha = 1, 2, \dots, \rho r - 1, \rho \nmid \alpha, r \nmid \alpha\}, \\V_3 &= \{r\alpha | \alpha = 1, 2, \dots, \rho q - 1, \rho \nmid \alpha, q \nmid \alpha\}, \\V_4 &= \{\rho q\alpha | \alpha = 1, 2, \dots, r - 1\}, \\V_5 &= \{\rho r\alpha | \alpha = 1, 2, \dots, q - 1\}, \\V_6 &= \{q r\alpha | \alpha = 1, 2, \dots, \rho - 1\}.\end{aligned}$$

Norm of each subsets are  $|V_1| = (q-1)(r-1)$ ,  $|V_2| = (q-1)(r-1)$ ,  $|V_3| = (\rho-1)(rq-1)$ ,  $|V_4| = (r-1)$ ,  $|V_5| = (q-1)$  and  $|V_6| = (\rho-1)$ , respectively.

Graph was constructed by using  $V_1$ ,  $V_2$ ,  $V_3$ ,  $V_4$ ,  $V_5$ , and  $V_6$  is below:

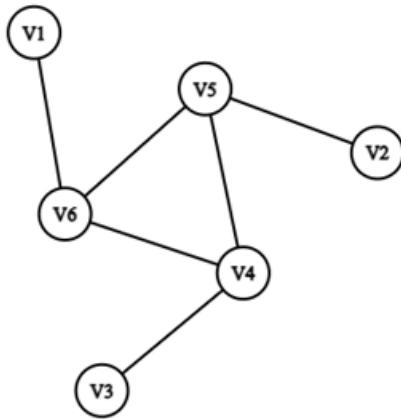


FIGURE 3. Structure of  $\Gamma(\mathbb{Z}_{\rho qr})$

In order to calculate Trinajstic index of  $\Gamma(\mathbb{Z}_{\rho qr})$  we must investigate these cases below:

**Case 1:** Considering the pair of sets  $V_1$  and  $V_2$ , where  $u \in V_1$  and  $v \in V_2$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_6| + |V_1|,$$

$$n_v = |V_5| + |V_2|.$$

$$\text{Thus, } (n_u - n_v)^2 = (|V_5| + |V_2| - (|V_6| + |V_1|))^2.$$

**Case 2:** Considering the pair of sets  $V_1$  and  $V_3$ , where  $u \in V_1$  and  $v \in V_3$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_6| + |V_1|,$$

$$n_v = |V_4| + |V_3|.$$

$$\text{Hence, } (n_u - n_v)^2 = (|V_6| + |V_1| - (|V_4| + |V_3|))^2.$$

**Case 3:** Considering the pair of sets  $V_1$  and  $V_4$ , where  $u \in V_1$  and  $v \in V_4$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = 0,$$

$$n_v = |V_3| + |V_5| + |V_2|.$$

$$\text{Therefore, } (n_u - n_v)^2 = (|V_3| + |V_5| + |V_2|)^2.$$

**Case 4:** Considering the pair of sets  $V_1$  and  $V_5$ , where  $u \in V_1$  and  $v \in V_5$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = 0,$$

$$n_v = |V_2| + |V_3| + |V_4|.$$

$$\text{Hence, } (n_u - n_v)^2 = (|V_2| + |V_3| + |V_4|)^2.$$

**Case 5:** Considering the pair of sets  $V_1$  and  $V_6$ , where  $u \in V_1$  and  $v \in V_6$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_6|,$$

$$n_v = |V_2| + |V_3| + |V_4| + |V_5| + |V_1|.$$

$$\text{Thus } (n_u - n_v)^2 = (|V_2| + |V_3| + |V_4| + |V_5| + |V_1| - |V_6|)^2.$$

**Case 6:** Considering the pair of sets  $V_2$  and  $V_3$ , where  $u \in V_2$  and  $v \in V_3$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_5| + |V_2|,$$

$$n_v = |V_4| + |V_3|.$$

$$\text{Therefore, } (n_u - n_v)^2 = (|V_5| + |V_2| - (|V_4| + |V_3|))^2.$$

**Case 7:** Considering the pair of sets  $V_2$  and  $V_4$ , where  $u \in V_2$  and  $v \in V_4$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = 0,$$

$$n_v = |V_3| + |V_1| + |V_6|.$$

$$\text{Hence, } (n_u - n_v)^2 = (|V_3| + |V_1| + |V_6|)^2.$$

**Case 8:** Considering the pair of sets  $V_2$  and  $V_5$ , where  $u \in V_2$  and  $v \in V_5$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_5|,$$

$$n_v = |V_1| + |V_2| + |V_3| + |V_4| + |V_6|.$$

$$\text{So, } (n_u - n_v)^2 = (|V_1| + |V_2| + |V_3| + |V_4| + |V_6| - |V_5|)^2.$$

**Case 9:** Considering the pair of sets  $V_2$  and  $V_6$ , where  $u \in V_2$  and  $v \in V_6$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = 0,$$

$$n_v = |V_1| + |V_3| + |V_4|.$$

$$\text{Accordingly, } (n_u - n_v)^2 = (|V_1| + |V_3| + |V_4|)^2.$$

**Case 10:** Considering the pair of sets  $V_3$  and  $V_4$ , where  $u \in V_3$  and  $v \in V_4$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_4|,$$

$$n_v = |V_1| + |V_2| + |V_3| + |V_5| + |V_6|.$$

$$\text{Thus, } (n_u - n_v)^2 = (|V_1| + |V_2| + |V_3| + |V_5| + |V_6| - |V_4|)^2.$$

**Case 11:** Considering the pair of sets  $V_3$  and  $V_5$ , where  $u \in V_3$  and  $v \in V_5$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = 0,$$

$$n_v = |V_1| + |V_2| + |V_6|.$$

$$\text{Hence, } (n_u - n_v)^2 = (|V_1| + |V_2| + |V_6|)^2.$$

**Case 12:** Considering the pair of sets  $V_3$  and  $V_6$ , where  $u \in V_3$  and  $v \in V_6$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = 0,$$

$$n_v = |V_1| + |V_2| + |V_5|.$$

$$\text{So, } (n_u - n_v)^2 = (|V_1| + |V_2| + |V_5|)^2.$$

**Case 13:** Considering the pair of sets  $V_4$  and  $V_5$ , where  $u \in V_4$  and  $v \in V_5$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_3| + |V_5|,$$

$$n_v = |V_2| + |V_4|.$$

$$\text{Thus } (n_u - n_v)^2 = (|V_3| + |V_5| - (|V_2| + |V_4|))^2.$$

**Case 14:** Considering the pair of sets  $V_4$  and  $V_6$ , where  $u \in V_4$  and  $v \in V_6$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_3| + |V_6|,$$

$$n_v = |V_1| + |V_4|.$$

$$\text{Therefore, } (n_u - n_v)^2 = (|V_3| + |V_6| - (|V_1| + |V_4|))^2.$$

**Case 15:** Considering the pair of sets  $V_5$  and  $V_6$ , where  $u \in V_5$  and  $v \in V_6$ , the values of  $n_u$  and  $n_v$  are described as follows:

$$n_u = |V_2| + |V_6|,$$

$$n_v = |V_1| + |V_5|.$$

$$\text{Hence, } (n_u - n_v)^2 = (|V_2| + |V_6| - (|V_1| + |V_5|))^2.$$

In this way, Trinajstic index of  $\Gamma(Z_{\rho qr})$  is

$$\begin{aligned} NT(\Gamma(Z_{\rho qr})) &= \sum_{\{u,v\} \in V(\Gamma(Z_{\rho qr}))} (n_u - n_v)^2 \\ &= |V_1||V_2|(|V_5| + |V_2| - (|V_6| + |V_1|))^2 + \\ &\quad |V_1||V_3|(|V_1| + |V_6| - (|V_3| + |V_4|))^2 + \\ &\quad |V_1||V_4|(|V_2| + |V_3| + |V_5|)^2 + |V_1||V_5|(|V_2| + |V_3| + |V_4|)^2 + \\ &\quad |V_1||V_6|(|V_1| + |V_2| + |V_3| + |V_4| + |V_5| - |V_6|)^2 + \\ &\quad |V_2||V_3|(|V_2| + |V_5| - (|V_3| + |V_4|))^2 + \\ &\quad |V_2||V_4|(|V_1| + |V_3| + |V_6|)^2 + \\ &\quad |V_2||V_5|(|V_1| + |V_2| + |V_3| + |V_4| + |V_6| - |V_5|)^2 + \\ &\quad |V_2||V_6|(|V_1| + |V_3| + |V_4|)^2 + \\ &\quad |V_3||V_4|(|V_1| + |V_2| + |V_3| + |V_5| + |V_6| - |V_4|)^2 + \\ &\quad |V_3||V_5|(|V_1| + |V_2| + |V_6|)^2 + \\ &\quad |V_3||V_3|(|V_1| + |V_2| + |V_5|)^2 + \\ &\quad |V_4||V_5|(|V_2| + |V_4| - (|V_3| + |V_5|))^2 + \\ &\quad |V_4||V_6|(|V_1| + |V_4| - (|V_3| + |V_6|))^2 + \\ &\quad |V_5||V_6|(|V_1| + |V_5| - (|V_2| + |V_6|))^2 \end{aligned} \tag{3.5}$$

Then Equation 3.5 will be

$$\begin{aligned}
 NT(\Gamma(\mathbb{Z}_{\rho qr})) = & (\rho - 1)^2(r - 1)(\rho q - 2q - \rho + qr + 1)^2 + \\
 & (q - 1)^2(r - 1)(\rho q - q - 2\rho + \rho r + 1)^2 + \\
 & (\rho - 1)^2(q - 1)(\rho r - 2r - \rho + qr + 1)^2 + \\
 & (q - 1)(r - 1)^2(\rho q - r - 2\rho + \rho r + 1)^2 + \\
 & (\rho - 1)(q - 1)^2(\rho r - 2r - q + qr + 1)^2 + \\
 & (\rho - 1)(r - 1)^2(\rho q - r - 2q + qr + 1)^2 + \\
 & (\rho - 1)(q - 1)(r - 1)(\rho q - q - 3r - \rho + \rho r + qr + 2)^2 + \\
 & (\rho - 1)(q - 1)(r - 1)(\rho q - 3q - r - \rho + \rho r + qr + 2)^2 + \\
 & (\rho - 1)(q - 1)(r - 1)(\rho q - q - r - 3\rho + \rho r + qr + 2)^2 + \\
 & r^2(\rho - q)^2(\rho - 1)(q - 1) + q^2(\rho - r)^2(\rho - 1)(r - 1) + \\
 & \rho^2(q - r)^2(q - 1)(r - 1) + (\rho - r)^2(\rho - 1)(q - 1)^2(q - 2)^2(r - 1) + \\
 & (q - r)^2(\rho - 1)^2(\rho - 2)^2(q - 1)(r - 1) + (\rho - q)^2(\rho - 1)(q - 1)(r - 1)^2(r - 2)^2
 \end{aligned}$$

□

Table 5.4 lists the results obtained for  $\Gamma(\mathbb{Z}_{\rho qr})$  for primes  $\rho < 10$ ,  $q < 10$  and  $r < 10$ .

#### 4. CONCLUSION

The Trinajstic index is a novel topological index that is one of the topological indexes to study on chemical graph theory, especially on chemical structure. The Trinajstic index could also be applicable on zero-divisor graphs except complete graph, star graph, path graph and cycle graph to improve theorems related to computer science and also graph theory too. As discussed in this paper, the Trinajstic index can be calculated analytically using prime numbers, without computational tools.

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#### 5. APPENDIX

Table 5.2: Results of  $\Gamma(\mathbb{Z}_{\rho q})$

$\rho$	$q$	$n = \rho q$	$NT$
2	2	4	0
2	3	6	2
2	5	10	36
2	7	14	150
2	11	22	810
2	13	26	1452
2	17	34	3600
2	19	38	5202

**Table 5.2 – continued from previous page**

$\rho$	$q$	$n = \rho q$	$NT$
2	23	46	9702
2	29	58	20412
2	31	62	25230
2	37	74	44100
2	41	82	60840
2	43	86	70602
2	47	94	93150
3	2	6	2
3	3	9	0
3	5	15	32
3	7	21	192
3	11	33	1280
3	13	39	2400
3	17	51	6272
3	19	57	9216
3	23	69	17600
3	29	87	37856
3	31	93	47040
3	37	111	83232
3	41	123	115520
3	43	129	134400
3	47	141	178112
5	2	10	36
5	3	15	32
5	5	25	0
5	7	35	96
5	11	55	1440
5	13	65	3072
5	17	85	9216
5	19	95	14112
5	23	115	28512
5	29	145	64512
5	31	155	81120
5	37	185	147456
5	41	205	207360
5	43	215	242592
5	47	235	324576
7	2	14	150
7	3	21	192
7	5	35	96

**Table 5.2 – continued from previous page**

$\rho$	$q$	$n = \rho q$	$NT$
7	7	49	0
7	11	77	960
7	13	91	2592
7	17	119	9600
7	19	133	15552
7	23	161	33792
7	29	203	81312
7	31	217	103680
7	37	259	194400
7	41	287	277440
7	43	301	326592
7	47	329	441600
11	2	22	810
11	3	33	1280
11	5	55	1440
11	7	77	960
11	11	121	0
11	13	143	480
11	17	187	5760
11	19	209	11520
11	23	253	31680
11	29	319	90720
11	31	341	120000
11	37	407	243360
11	41	451	360000
11	43	473	430080
11	47	517	596160
13	2	26	1452
13	3	39	2400
13	5	65	3072
13	7	91	2592
13	11	143	480
13	13	169	0
13	17	221	3072
13	19	247	7776
13	23	299	26400
13	29	377	86016
13	31	403	116640
13	37	481	248832
13	41	533	376320

**Table 5.2 – continued from previous page**

$\rho$	$q$	$n = \rho q$	$NT$
13	43	559	453600
13	47	611	638112
17	2	34	3600
17	3	51	6272
17	5	85	9216
17	7	119	9600
17	11	187	5760
17	13	221	3072
17	17	289	0
17	19	323	1152
17	23	391	12672
17	29	493	64512
17	31	527	94080
17	37	629	230400
17	41	697	368640
17	43	731	454272
17	47	799	662400
19	2	38	5202
19	3	57	9216
19	5	95	14112
19	7	133	15552
19	11	209	11520
19	13	247	7776
19	17	323	1152
19	19	361	0
19	23	437	6336
19	29	551	50400
19	31	589	77760
19	37	703	209952
19	41	779	348480
19	43	817	435456
19	47	893	649152
23	2	46	9702
23	3	69	17600
23	5	115	28512
23	7	161	33792
23	11	253	31680
23	13	299	26400
23	17	391	12672
23	19	437	6336

**Table 5.2 – continued from previous page**

$\rho$	$q$	$n = \rho q$	$NT$
23	23	529	0
23	29	667	22176
23	31	713	42240
23	37	851	155232
23	41	943	285120
23	43	989	369600
23	47	1081	582912
29	2	58	20412
29	3	87	37856
29	5	145	64512
29	7	203	81312
29	11	319	90720
29	13	377	86016
29	17	493	64512
29	19	551	50400
29	23	667	22176
29	29	841	0
29	31	899	3360
29	37	1073	64512
29	41	1189	161280
29	43	1247	230496
29	47	1363	417312
31	2	62	25230
31	3	93	47040
31	5	155	81120
31	7	217	103680
31	11	341	120000
31	13	403	116640
31	17	527	94080
31	19	589	77760
31	23	713	42240
31	29	899	3360
31	31	961	0
31	37	1147	38880
31	41	1271	120000
31	43	1333	181440
31	47	1457	353280
37	2	74	44100
37	3	111	83232
37	5	185	147456

**Table 5.2 – continued from previous page**

$\rho$	$q$	$n = \rho q$	$NT$
37	7	259	194400
37	11	407	243360
37	13	481	248832
37	17	629	230400
37	19	703	209952
37	23	851	155232
37	29	1073	64512
37	31	1147	38880
37	37	1369	0
37	41	1517	23040
37	43	1591	54432
37	47	1739	165600
41	2	82	60840
41	3	123	115520
41	5	205	207360
41	7	287	277440
41	11	451	360000
41	13	533	376320
41	17	697	368640
41	19	779	348480
41	23	943	285120
41	29	1189	161280
41	31	1271	120000
41	37	1517	23040
41	41	1681	0
41	43	1763	6720
41	47	1927	66240
43	2	86	70602
43	3	129	134400
43	5	215	242592
43	7	301	326592
43	11	473	430080
43	13	559	453600
43	17	731	454272
43	19	817	435456
43	23	989	369600
43	29	1247	230496
43	31	1333	181440
43	37	1591	54432
43	41	1763	6720

**Table 5.2 – continued from previous page**

$\rho$	$q$	$n = \rho q$	$NT$
43	43	1849	0
43	47	2021	30912
47	2	94	93150
47	3	141	178112
47	5	235	324576
47	7	329	441600
47	11	517	596160
47	13	611	638112
47	17	799	662400
47	19	893	649152
47	23	1081	582912
47	29	1363	417312
47	31	1457	353280
47	37	1739	165600
47	41	1927	66240
47	43	2021	30912
47	47	2209	0

Table 5.3: Results of  $\Gamma(\mathbb{Z}_{\rho^2 q})$ 

$\rho$	$q$	$\rho^2$	$n = \rho^2 q$	$NT$
2	2	4	8	2
2	3	4	12	116
2	5	4	20	600
2	7	4	28	1836
2	11	4	44	8100
2	13	4	52	13896
2	17	4	68	32736
2	19	4	76	46548
3	2	9	18	1062
3	3	9	27	300
3	5	9	45	10404
3	7	9	63	26112
3	11	9	99	95832
3	13	9	117	156756
3	17	9	153	348012
3	19	9	171	485256
5	2	25	50	43860
5	3	25	75	95960
5	5	25	125	28880
5	7	25	175	561960
5	11	25	275	1843320
5	13	25	325	2957760
5	17	25	425	6470160
5	19	25	475	9002520
7	2	49	98	491946
7	3	49	147	966336
7	5	49	245	2107140
7	7	49	343	423612
7	11	49	539	11130000
7	13	49	637	17509716
7	17	49	833	38036796
7	19	49	931	53087328
11	2	121	242	12997710
11	3	121	363	23982200
11	5	121	605	42850500
11	7	121	847	62037360
11	11	121	1331	13069100
11	13	121	1573	174942900
11	17	121	2057	349767660

**Table 5.3 – continued from previous page**

$\rho$	$q$	$\rho^2$	$n = \rho^2 q$	$NT$
11	19	121	2299	483076440
13	2	169	338	43707612
13	3	169	507	80297256
13	5	169	845	139324224
13	7	169	1183	190351512
13	11	169	1859	320583432
13	13	169	2197	44974800
13	17	169	2873	782036112
13	19	169	3211	1058991336
17	2	289	578	305388816
17	3	289	867	563382176
17	5	289	1445	966976320
17	7	289	2023	1265474016
17	11	289	3179	1762029600
17	13	289	3757	2067512256
17	17	289	4913	319615232
17	19	289	5491	3857328288
19	2	361	722	682331382
19	3	361	1083	1263762504
19	5	361	1805	2177294436
19	7	361	2527	2838441312
19	11	361	3971	3787845624
19	13	361	4693	4268235924
19	17	361	6137	5720724972
19	19	361	6859	715825836

Table 5.4: Results of  $\Gamma(\mathbb{Z}_{\rhoqr})$ 

$\rho$	$q$	$r$	$n = \rhoqr$	$NT$
2	2	2	8	2
2	2	3	12	116
2	2	5	20	600
2	2	7	28	1836
2	3	2	12	116
2	3	3	18	1062
2	3	5	30	14922
2	3	7	42	48980
2	5	2	20	600
2	5	3	30	14922
2	5	5	50	43860
2	5	7	70	273278
2	7	2	28	1836
2	7	3	42	48980
2	7	5	70	273278
2	7	7	98	491946
3	2	2	12	116
3	2	3	18	1062
3	2	5	30	14922
3	2	7	42	48980
3	3	2	18	1062
3	3	3	27	300
3	3	5	45	10404
3	3	7	63	26112
3	5	2	30	14922
3	5	3	45	10404
3	5	5	75	95960
3	5	7	105	734912
3	7	2	42	48980
3	7	3	63	26112
3	7	5	105	734912
3	7	7	147	966336
5	2	2	20	600
5	2	3	30	14922
5	2	5	50	43860
5	2	7	70	273278
5	3	2	30	14922
5	3	3	45	10404
5	3	5	75	95960

**Table 5.4 – continued from previous page**

$\rho$	$q$	$r$	$n = \rhoqr$	$NT$
5	3	7	105	734912
5	5	2	50	43860
5	5	3	75	95960
5	5	5	125	28880
5	5	7	175	561960
5	7	2	70	273278
5	7	3	105	734912
5	7	5	175	561960
5	7	7	245	2107140
7	2	2	28	1836
7	2	3	42	48980
7	2	5	70	273278
7	2	7	98	491946
7	3	2	42	48980
7	3	3	63	26112
7	3	5	105	734912
7	3	7	147	966336
7	5	2	70	273278
7	5	3	105	734912
7	5	5	175	561960
7	5	7	245	2107140
7	7	2	98	491946
7	7	3	147	966336
7	7	5	245	2107140
7	7	7	343	423612

**REFERENCES**

- [1] Anderson, D. F., & Badawi, A. (2008). On the zero-divisor graph of a ring. *Communications in Algebra*, 36(8), 3073–3092.
- [2] Anderson, D. F., Axtell, M. C., & Stickles, J. A. (2011). Zero-divisor graphs in commutative rings. In *Commutative algebra: Noetherian and non-Noetherian perspectives* (pp. 23–45). Springer.
- [3] Balaban, A. T. (2013). Chemical graph theory and the Sherlock Holmes principle. *International Journal for Philosophy of Chemistry*, 9(1), 107–137.
- [4] Beck, I. (1988). Coloring of commutative rings. *Journal of Algebra*, 116(1), 208–226.
- [5] Bondy, J. A., & Murty, U. S. R. (1976). *Graph theory with applications* (Vol. 290). Macmillan.
- [6] Brezovnik, S., & Tratnik, N. (2018). New methods for calculating the degree distance and the Gutman index. *arXiv preprint*. arXiv:1809.02358.
- [7] Coykendall, J., Sather-Wagstaff, S., Sheppardson, L., & Spiroff, S. (2012). On zero divisor graphs. *Progress in Commutative Algebra*, 2, 241–299.
- [8] Dehgardi, N., & Azari, M. (2020). More on Mostar index. *Applied Mathematics E-Notes*, 20, 316–322.
- [9] Došlić, T., Martinjak, I., Škrekovski, R., Tipurić Spužević, S., & Zubac, I. (2018). Mostar index. *Journal of Mathematical Chemistry*, 56, 2995–3013.

- [10] Furtula, B., & Gutman, I. (2015). A forgotten topological index. *Journal of Mathematical Chemistry*, 53(4), 1184–1190.
- [11] Furtula, B. (2022). Trinajstić index. *Discrete Mathematics Letters*, 9, 100–106.
- [12] García-Domenech, R., Gálvez, J., de Julián-Ortiz, J. V., & Pogliani, L. (2008). Some new trends in chemical graph theory. *Chemical Reviews*, 108(3), 1127–1169.
- [13] Gould, R. (2012). *Graph theory*. Courier Corporation.
- [14] Gutman, I. (1994). A formula for the Wiener number of trees and its extension to graphs containing cycles. *Graph Theory Notes of New York*, 27, 9–15.
- [15] Gutman, I. (2013). Degree-based topological indices. *Croatica Chemica Acta*, 86(4), 351–361.
- [16] Gutman, I. (2021). Geometric approach to degree-based topological indices: Sombor indices. *MATCH Communications in Mathematical and Computer Chemistry*, 86(1), 11–16.
- [17] Gutman, I., & Trinajstić, N. (1972). Graph theory and molecular orbitals: Total  $\phi$ -electron energy of alternant hydrocarbons. *Chemical Physics Letters*, 17(4), 535–538.
- [18] Gutman, I., Gürsoy, N. K., Gürsoy, A., & Ülker, A. (2023). New bounds on Sombor index. *Communications in Combinatorics and Optimization*, 8(2), 305–311.
- [19] Gürsoy, A., Gürsoy, N. K., & Ülker, A. (2022). Computing forgotten topological index of zero-divisor graphs of commutative rings. *Turkish Journal of Mathematics*, 46(5), 1845–1863.
- [20] Hayat, S., & Imran, M. (2014). Computation of topological indices of certain networks. *Applied Mathematics and Computation*, 240, 213–228.
- [21] Heydari, A. (2010). On the modified Schultz index of C<sub>4</sub>C<sub>8</sub> (s) nanotubes and nanotorus. *Digest Journal of Nanomaterials and Biostuctures*, 5(1), 51–56.
- [22] Ivanciu, 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] Kircali Gürsoy, N., Ülker, A., & Gürsoy, A. (2022). Independent domination polynomial of zero-divisor graphs of commutative rings. *Soft Computing*, 26(15), 6989–6997.
- [24] Kızıltırnak, G. O. (2022). Bounds for some distance-based and degree-distance-based topological indices. *Contributions to Mathematics*, 6, 45–49.
- [25] Klavžar, S., & Gutman, I. (1996). A comparison of the Schultz molecular topological index with the Wiener index. *Journal of Chemical Information and Computer Sciences*, 36(5), 1001–1003.
- [26] Konstantinova, E. V., Skorobogatov, V. A., & Vidyuk, M. V. (2003). Applications of information theory in chemical graph theory. *Indian Journal of Chemistry, Section A*, 42(6), 1227–1240.
- [27] Merris, R. (2011). *Graph theory*. Wiley.
- [28] Randić, M. (1975). Characterization of molecular branching. *Journal of the American Chemical Society*, 97(23), 6609–6615.
- [29] Randić, M., & Trinajstić, N. (1994). Notes on some less known early contributions to chemical graph theory. *Croatica Chemica Acta*, 67(1), 1–35.
- [30] Randić, M. (2008). On history of the Randić index and emerging hostility toward chemical graph theory. *MATCH Communications in Mathematical and Computer Chemistry*, 59(1), 5–124.
- [31] Rouvray, D. H. (1987). The modeling of chemical phenomena using topological indices. *Journal of Computational Chemistry*, 8(4), 470–480.
- [32] Rouvray, D. H. (2002). The rich legacy of half a century of the Wiener index. In D. Bonchev & D. H. Rouvray (Eds.), *Chemical graph theory: Introduction and fundamentals* (pp. 16–37). Abacus Press.
- [33] Schultz, H. P. (1989). Topological organic chemistry. Part 1: Graph theory and topological indices of alkanes. *Journal of Chemical Information and Computer Sciences*, 29(3), 227–228.
- [34] Su, G., Xiong, L., Gutman, I., & Xu, L. (2016). Reciprocal product-degree distance of graphs. *Filomat*, 30(8), 2217–2231.
- [35] Todeschini, R., & Consonni, V. (2008). *Handbook of molecular descriptors*. Wiley.
- [36] Tutte, W. T. (2001). *Graph theory* (Vol. 21). Cambridge University Press.
- [37] Van Steen, M. (2010). *Graph theory and complex networks: An introduction*. Maarten van Steen.

- [38] Wiener, H. (1947). Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69(1), 17–20.
- [39] Zhang, P., & Chartrand, G. (2006). *Introduction to graph theory*. McGraw-Hill.
- [40] Zhou, B. (2004). Zagreb indices. *MATCH Communications in Mathematical and Computer Chemistry*, 52(1), 113–118.
- [41] Zhou, B., Cai, X., & Trinajstić, N. (2008). On Harary index. *Journal of Mathematical Chemistry*, 44(4), 611–618.

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