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Computing Topological Descriptors of Prime Ideal Sum Graphs of Commutative Rings

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Abstract: Let $n \geq 1$ be a fixed integer. The main objective of this paper is to compute some topological indices and coindices that are related to the graph complement of the prime ideal sum (PIS) graph of \mathbb{Z}_n , where $n = p^\alpha, p^2q, p^2q^2, pqr, p^3q, p^2qr$, and $pqrs$ for the different prime integers p, q, r , and s . Moreover, we construct M -polynomials and CoM -polynomials using the PIS -graph structure of \mathbb{Z}_n to avoid the difficulty of computing the descriptors via formulas directly. Furthermore, we present a geometric comparison for representations of each surface obtained by M -polynomials and CoM -polynomials. Finally, we discuss the applicability of algebraic graphs to chemical graph theory.

Keywords: topological index; topological coindex; prime ideal sum (PIS) graph; complement of a graph; M -polynomial; CoM -polynomial

MSC: 05C07; 05C09; 05C25; 05C31; 05C62



Citation: Öztürk Sözen, E.; Alsuraiheed, T.; Abdioğlu, C.; Ali, S. Computing Topological Descriptors of Prime Ideal Sum Graphs of Commutative Rings. *Symmetry* **2023**, *15*, 2133. <https://doi.org/10.3390/sym15122133>

Academic Editors: Ismail Naci Cangul, Kinkar Chandra Das, Ahmet Sinan Cevik, Michel Planat and Sergei D. Odintsov

Received: 23 September 2023
Revised: 17 November 2023
Accepted: 24 November 2023
Published: 30 November 2023



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1. Introduction

Graph theory is a mathematical modeling method that explains the way objects are related to each other by connecting them with graphs called edges. Arthur Cayley [1] played a pivotal role in the resurgence of graph theory applications within the field of chemistry, ultimately giving birth to what we now know as chemical graph theory [2]. In this branch, the atoms organizing a molecule are considered as points; bonds between atoms are considered as edges. Then, the concept of a topological index becomes involved, whose final value is obtained from the values extracted from the molecular graph model. Topological indices are formulas that enable us to predict the physicochemical data of molecules, obtained through long experimental processes with mathematical calculations. In this way, it is possible to gain recoup losses arising from parameters such as time, equipment, budget, and environment during the experimental process. Topological indices can be decomposed into distance- and degree-based indices. The Wiener index [3], Zagreb indices [4], Randic index [5], Balaban index [6], and Hosoya [7] and Forgotten topological indices [8] are the leading ones. While taking into account the number of other vertices to which a vertex is connected for degree-based indices, distance-based indices take the shortest path between two points as a basis. For novel and further properties of topological indices, we also refer the reader to [9–12], where further references can be found. It may not always be easy or even possible to make formulary calculations among hundreds of topological indices. To eliminate this difficulty and also in order to have information about the topological surface, a computing method has already been developed using algebraic polynomials. For instance, in the domain of distance-based topological indices, the Wiener polynomial is a general polynomial whose derivatives at 1 yield Wiener and

hyper-Wiener indices [13]. It can be predicted that finding the shortest path between any two points in a complex graph structure may not always be easy. Most of the time, the need to use algorithms may be felt. Similarly, for the degree-based topological indices, M- and NM-polynomials were defined in [14] and [15], respectively, and given as follows:

$$M(G; x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j,$$

where m_{ij} , $i, j \geq 1$, and the number of edges $uv \in E(G)$ such that $\{(d(u), d(v)) = \{i, j\}\}$ for the degrees $d(u)$ and $d(v)$ of u, v in G . In addition,

$$NM(G; x, y) = \sum_{i \leq j} n_{ij}(G) x^i y^j,$$

where n_{ij} , $i, j \geq 1$, and the number of edges $uv \in E(G)$ such that $\{(\delta(u), \delta(v)) = \{i, j\}\}$ for the neighborhood degrees $\delta(u)$ and $\delta(v)$ of u, v in G .

Over time, in parallel with the topological indices, topological coindices, calculated according to the values taken from the complement of the molecular graph, have been added to the literature (see [12,16] for details). The complement graph \overline{G} was obtained by plotting the relationship between non-adjacent pairs of points of a graph G [16]. The indices calculated based on this new structure are also called topological coindices, and just as the others, it is possible to classify them based on degree and distance. For example, the first and the second Zagreb coindices were introduced by Doslic in [17] as follows:

$$\overline{M}_1(G) = \sum_{ab \in E(\overline{G})} (d(a) + d(b))$$

and

$$\overline{M}_2(G) = \sum_{ab \in E(\overline{G})} (d(a)d(b)),$$

where the degrees $d(a)$ and $d(b)$ indicate the number of vertices that are non-adjacent to a and b , respectively. Later, the multiplicative Zagreb coindices [18], forgotten topological coindex [19], second modified Zagreb coindex [20], redefined third Zagreb coindex [20], Randic coindex [20], inverse Randic coindex [20], symmetric division coindex [20], harmonic coindex [20], inverse sum indeg coindex [20], and augmented Zagreb coindex [20] were also defined and studied. In 2022, Kirmani et al. [20] introduced and studied CoM-polynomials as an alternative way to compute topological coindices. Additionally, some recent studies can be presented as examples of the applications of degree-based topological indices computed via the mentioned polynomials in QSPR analysis (see [21–24] and references therein).

Topological indices and algebraic graph theory share a common focus on the analysis and representation of graphs. Topological indices offer a distinctive set of numerical measurements derived from graph topology. On the other hand, algebraic graph theory provides mathematical tools and concepts that enable the analysis and comprehension of graph features. These tools are effectively utilized to investigate and gain insights into topological indices, thereby establishing a mutual relationship between the two. Graphs with commutative rings are employed in robotics, information and communication theory, elliptic curve cryptography, physics, and statistics. The constructed graphs from algebraic structures exhibit remarkable properties that showcase their high degree of symmetry. These properties establish a significant connection between chemical graph theory and network utilized in parallel computing. The ring structure's graphs have also been applied in molecular graphs and the structures of genetic code [25]. Nowadays, studies on the zero divisor graph of the ring \mathbb{Z}_n are a trending field in spectral and chemical graph theory (see [26–29] for details). Studies on these topics in the literature motivated us to study computing different descriptors with respect to a prime ideal sum graph. The prime ideal sum graph of a commutative ring was defined in [30]. For a commutative ring R with identity, the prime ideal sum graph of R is a graph whose vertices are nonzero proper

ideals of R , and two distinct vertices I and J are adjacent if and only if $I + J$ is a prime ideal of R . They studied some connections between the graph-theoretic properties of this graph and some algebraic properties of rings (see [30] for more details).

The main goals of the present paper are to compute some topological indices first Zagreb index ($M_1(G)$), second Zagreb index ($M_2(G)$), second modified Zagreb index ($mM_2(G)$), redefined third Zagreb index ($RezG_3$), forgotten topological index ($F(G)$), symmetric division index ($SDD(G)$), harmonic index ($H(G)$), inverse sum indeg index ($I(G)$), and augmented Zagreb index ($A(G)$) and the topological coindex version each of them, which are related to the complement of the PIS graph of \mathbb{Z}_n for $n = p^\alpha, p^2q, p^2q^2, pqr, p^3q, p^2qr, pqrs$, where p, q, r , and s are distinct primes. Furthermore, we construct M -polynomials and CoM -polynomials using the PIS-graph structure of \mathbb{Z}_n to avoid the difficulty of calculating descriptors via formulas directly. Furthermore, we discuss applications of the M -polynomials and CoM -polynomials of molecular graphs in order to shed light on the topological structures of the taken molecules. The paper ends with conclusions and directions for future research.

2. Motivation behind Topological Indices over Algebraic Graphs

In chemistry, group theory is used to study the symmetries and the crystal structures of objects whenever an object or a system property is invariant under transformation. The idea of constructing a graph from groups was advanced by Arthur Cayley, since an algebraic structure is essential for the development of chemical systems as well as the study of many chemical properties of molecules contained within these structures. The study of graphs from rings commences with the exploration of the thoroughly-researched zero-divisor graphs derived from commutative rings [31]. The other well-studied graphs produced from rings can be listed as annihilating ideal graphs [32], comaximal graphs [33,34], Cayley graphs [35], prime ideal sum graphs, total graph [36], etc.

Since topological indices are the numerical quantity of a network and are invariant under graph isomorphisms, researchers are interested in examining the physical properties and symmetries of algebraic structures through graph representations, similar to those in chemistry. In addition, graphs constructed from rings are finite structures, and finite rings and fields have received a significant amount of focus for their applications in cryptography and coding theory [37–39]. In [40–42], the authors computed vertex-based eccentric and edge-based topological indices of zero-divisor graphs of $\mathbb{Z}_{pq} \times \mathbb{Z}_r$, where p, q , and r are primes. They pointed out the benefits of these indices in understanding the characteristics of different physical structures such as carbon nanostructures, hexagonal belts and chains, fullerenes and nanocones, structure boiling points, and the relationships of various alkanes. Moreover, they have significance in estimating and troubleshooting computer network problems and developing efficient physical structure in robotics.

In particular, in a recent study (2023) entitled “Applications on Topological Indices of Zero-Divisor Graph Associated with Commutative Rings”, it was declared that computed values for topological indices over algebraic graphs help understand the characteristics of various symmetric physical structures of finite commutative rings and have received significant focus for their applications to cryptography, coding theory, robotics, and mechanics [43,44]. These predictions are also supported by the following recent articles, as the graphs constructed from rings were highly symmetric [45–47]. Another article published in Nature Communications [48], entitled “Algebraic Graph-Assisted Bidirectional Transformers for Molecular Property Prediction”, shows promise that algebraic graph theory with the applications of topological indices will gain a place in interdisciplinary applications in the near future. Our prediction is that topological indices will be active in the optimization of applications/systems developed using algebraic graphs [49].

Inspired by the abovementioned studies, in Section 6, we contribute to this literature by computing prime ideal sum graphs of commutative rings. Precisely, we discuss some applications of algebraic graphs to chemical graph theory.

3. Preliminaries

First, let us list the related notations used in this paper ($i \leq j$).

$$\begin{aligned}
 n_i &= |V_i| \text{ for } V_i = \{a \in V(G) \mid d(a) = i\} \\
 m_{ij} &= |E_{ij}| \\
 E_{ij} &= \{ab \in E(G) \mid d(a) = i \text{ and } d(b) = j\} \\
 \bar{m}_{ij} &= |\bar{E}_{ij}| \text{ for } \bar{E}_{ij} = \{ab \in E(\bar{G}) \mid d(a) = i \text{ and } d(b) = j\}.
 \end{aligned}$$

The following lemma is used to construct the CoM-polynomial of a commutative ring, which is designed via the complement graph \bar{G} of the related commutative ring, given in [50]. Moreover, the prime ideal sum graph of a ring R is denoted by $PIS(R)$.

Lemma 1. *Let G be a connected graph of order n . Then, the statement given below is provided.*

$$\bar{m}_{ij} = |\bar{E}_{ij}| = \begin{cases} \frac{n_i(n_i-1)}{2} - m_{ii} & \text{for } i = j \\ n_i n_j - m_{ij} & \text{for } i < j. \end{cases}$$

The concept of the CoM-polynomial of the two variables x, y is defined as follows [20]:

$$CoM(G; x, y) = \bar{M}(G; x, y) = \sum_{i \leq j} \bar{m}_{ij}(G) x^i y^j,$$

where $\bar{m}_{ij}, i, j \geq 1$, and the number of edges $uv \notin E(G)$ such that $(d(a), d(b)) = (i, j)$.

Finally, we present the operators that will be used in the next section whenever presenting the polynomials corresponding to topological descriptors:

$$\begin{aligned}
 D_x &= x \frac{\partial(h(x,y))}{\partial x}, & S_x &= \int_0^x \frac{h(t,y)}{t} dt, & J(h(x,y)) &= h(x,x), \\
 D_y &= y \frac{\partial(h(x,y))}{\partial y}, & S_y &= \int_0^y \frac{h(x,t)}{t} dt, & Q_k(h(x,y)) &= x^k h(x,y).
 \end{aligned}$$

4. Materials and Modeling

In this section, we present the formulas of topological indices and coindices as tables (see Tables 1 and 2) that we use for calculating numeric values as follows:

Table 1. Topological indices.

Topological Index	Formula	Polynomial Form $h(x, y) = M(x, y)$
First Zagreb Index: M_1	$\sum_{ab \in E} [d(a) + d(b)]$	$(D_x + D_y)(h(x, y)) _{(1,1)}$
Second Zagreb Index: M_2	$\sum_{ab \in E} [d(a)d(b)]$	$(D_x D_y)(h(x, y)) _{(1,1)}$
Second Modified Zagreb Index: mM_2	$\sum_{ab \in E} \frac{1}{[d(a)d(b)]}$	$(S_x S_y)(h(x, y)) _{(1,1)}$
Redefined Third Zagreb Index: $ReZG_3$	$\sum_{ab \in E} (d(a)d(b))[d(a) + d(b)]$	$(D_x D_y)(D_x + D_y)(h(x, y)) _{(1,1)}$
Forgotten Topological Index: F	$\sum_{ab \in E} [d^2(a) + d^2(b)]$	$(D_x^2 + D_y^2)(h(x, y)) _{(1,1)}$
Randic Index: R_k	$\sum_{ab \in E} [d(a)d(b)]^k$	$(D_x^k + D_y^k)(h(x, y)) _{(1,1)}$
Inverse Randic Index: RR_k	$\sum_{ab \in E} \frac{1}{[d(a)d(b)]^k}$	$(S_x^k S_y^k)(h(x, y)) _{(1,1)}$
Symmetric Division Index: SDD	$\sum_{ab \in E} \frac{[d^2(a) + d^2(b)]}{[d(a)d(b)]}$	$(D_x S_y + S_x D_y)(h(x, y)) _{(1,1)}$
Harmonic Index: H	$\sum_{ab \in E} \frac{2}{[d(a)d(b)]}$	$(2S_x J)(h(x, y)) _{x=1}$
Inverse Sum Indeg Index: I	$\sum_{ab \in E} \frac{[d(a)d(b)]}{[d(a) + d(b)]}$	$(S_x J D_x D_y)(h(x, y)) _{x=1}$
Augmented Zagreb Index: A	$\sum_{ab \in E} \frac{[d(a)d(b)]}{[d(a) + d(b) - 2]^3}$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(h(x, y)) _{x=1}$

Table 2. Topological coindices.

Topological Coindex	Formula	Polynomial Form $h(x, y) = CoM(x, y)$
First Zagreb Coindex: \overline{M}_1	$\sum_{ab \notin E} [d(a) + d(b)]$	$(D_x + D_y)(h(x, y)) _{(1,1)}$
Second Zagreb Coindex: \overline{M}_2	$\sum_{ab \notin E} [d(a)d(b)]$	$(D_x D_y)(h(x, y)) _{(1,1)}$
Second Modified Zagreb Coindex: $m\overline{M}_2$	$\sum_{ab \notin E} \frac{1}{[d(a)d(b)]}$	$(S_x S_y)(h(x, y)) _{(1,1)}$
Redefined Third Zagreb Coindex: \overline{ReZG}_3	$\sum_{ab \notin E} (d(a)d(b))[d(a) + d(b)]$	$(D_x D_y)(D_x + D_y)(h(x, y)) _{(1,1)}$
Forgotten Topological Coindex: \overline{F}	$\sum_{ab \notin E} [d^2(a) + d^2(b)]$	$(D_x^2 + D_y^2)(h(x, y)) _{(1,1)}$
Randic Coindex: \overline{R}_k	$\sum_{ab \notin E} [d(a)d(b)]^k$	$(D_x^k + D_y^k)(h(x, y)) _{(1,1)}$
Inverse Randic Coindex: \overline{RR}_k	$\sum_{ab \notin E} \frac{1}{[d(a)d(b)]^k}$	$(S_x^k S_y^k)(h(x, y)) _{(1,1)}$
Symmetric Division Coindex: \overline{SDD}	$\sum_{ab \notin E} \frac{[d^2(a) + d^2(b)]}{[d(a)d(b)]}$	$(D_x S_y + S_x D_y)(h(x, y)) _{(1,1)}$
Harmonic Coindex: \overline{H}	$\sum_{ab \notin E} \frac{2}{[d(a)d(b)]}$	$(2S_x J)(h(x, y)) _{x=1}$
Inverse Sum Indeg Coindex: \overline{I}	$\sum_{ab \notin E} \frac{[d(a)d(b)]}{[d(a) + d(b)]}$	$(S_x J D_x D_y)(h(x, y)) _{x=1}$
Augmented Zagreb Coindex: \overline{A}	$\sum_{ab \notin E} \frac{[d(a)d(b)]}{[d(a) + d(b) - 2]^3}$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(h(x, y)) _{x=1}$

5. Polynomial Forms and Topological Descriptors of Algebraic Graphs

5.1. M-Polynomials and CoM-Polynomials of Some Commutative Rings

The first main result of this paper is the following theorem.

Theorem 1. Let p be a prime integer and α be an integer with $\alpha \geq 2$. Then, the M-polynomial and CoM-polynomial of \mathbb{Z}_{p^α} have the forms

$$M(\mathbb{Z}_{p^\alpha}; x, y) = (\alpha - 2)xy^{\alpha-2}, \alpha \geq 2$$

$$CoM(\mathbb{Z}_{p^\alpha}; x, y) = 0, \alpha \geq 2.$$

Proof. Let us list all ideals of \mathbb{Z}_{p^α} . Then, we have $\{0\}, u_{\alpha-1} = p^{\alpha-1}\mathbb{Z}_{p^\alpha}, u_{\alpha-2} = p^{\alpha-2}\mathbb{Z}_{p^\alpha}, \dots, u_3 = p^3\mathbb{Z}_{p^\alpha}, u_2 = p^2\mathbb{Z}_{p^\alpha}, u_1 = p\mathbb{Z}_{p^\alpha}, \mathbb{Z}_{p^\alpha}$. Note that $p\mathbb{Z}_{p^\alpha}$ is a prime ideal of \mathbb{Z}_{p^α} . Taking into account the PIS graph over \mathbb{Z}_{p^α} , it can be seen that $p\mathbb{Z}_{p^\alpha}$ is adjacent to $p^{\alpha-1}\mathbb{Z}_{p^\alpha}, p^{\alpha-2}\mathbb{Z}_{p^\alpha}, \dots, p^2\mathbb{Z}_{p^\alpha}$ as \mathbb{Z}_{p^α} is local, and thus the sum of these ideals is equal to \mathbb{Z}_{p^α} . Consider the following graph representation of \mathbb{Z}_{p^α} in Figure 1:

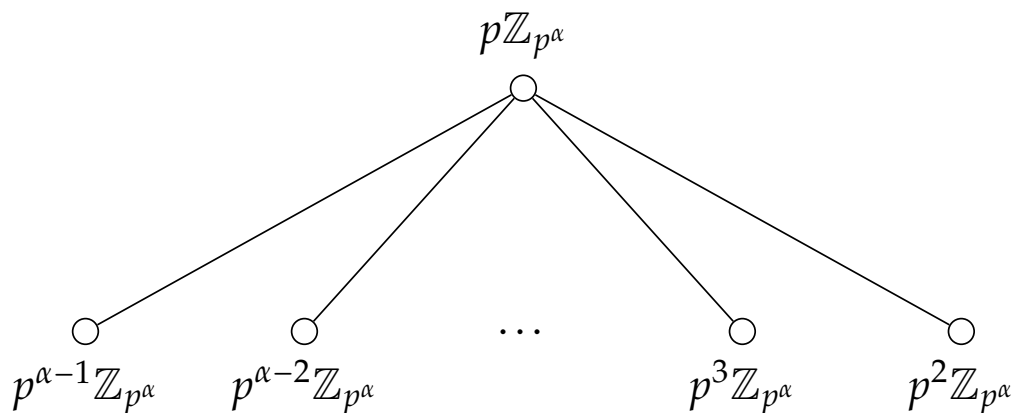


Figure 1. Prime ideal sum graph of \mathbb{Z}_{p^α} .

From the PIS-graph structure of \mathbb{Z}_{p^α} , we obtain:

$$d(u_1) = \alpha - 2, d(u_2) = d(u_3) = \dots = d(u_{\alpha-1}) = 1$$

using the concept of the degree of a vertex. It follows that $n_1 = \alpha - 2$ and $n_{\alpha-2} = 1$ using the notations given at the beginning of the Preliminaries section by vertex partition and by the edge-partition technique.

$$m_{1\alpha-2} = \alpha - 2, \quad \bar{m}_{1\alpha-2} = n_1 n_{\alpha-2} - m_{1\alpha-2} = (\alpha - 2) \times 1 - (\alpha - 2) = 0.$$

Hence,

$$M(\mathbb{Z}_{p^2q}; x, y) = \sum_{i \leq j} m_{ij} x^i y^j = (\alpha - 2) x y^{\alpha-2},$$

$$CoM(\mathbb{Z}_{p^2q}; x, y) = \sum_{i \leq j} \bar{m}_{ij} x^i y^j = 0. \quad \square$$

Theorem 2. Let p and q be distinct prime integers. Then, the M -polynomial and CoM -polynomial of \mathbb{Z}_{p^2q} have the forms

$$M(\mathbb{Z}_{p^2q}; x, y) = x y^3 + x^2 y^2 + 2 x^2 y^3,$$

$$CoM(\mathbb{Z}_{p^2q}; x, y) = 0.$$

Proof. Let us consider the ideals $u_1 = p\mathbb{Z}_n, u_2 = q\mathbb{Z}_n, u_3 = pq\mathbb{Z}_n, u_4 = p^2\mathbb{Z}_n$ for $n = p^2q$. Then, $PIS(\mathbb{Z}_n)$ is given in Figure 2. Since $d(u_1) = 2, d(u_2) = 1, d(u_3) = 3, d(u_4) = 2$, we have $n_1 = 1, n_2 = 1, n_3 = 1$ by vertex partition. Therefore, we obtain:

$$m_{13} = 1, \quad \bar{m}_{13} = n_1 n_3 - m_{13} = 1 - 1 = 0$$

$$m_{22} = 1, \quad \bar{m}_{22} = \frac{n_2(n_2-1)}{2} - m_{22} = \frac{2 \times 1}{2} - 1 = 0$$

$$m_{23} = 2, \quad \bar{m}_{23} = n_2 n_3 - m_{23} = 2 \times 1 - 2 = 0$$

using the edge-partition technique. Hence, the mentioned polynomials are obtained as follows:

$$M(\mathbb{Z}_{p^2q}; x, y) = \sum_{i \leq j} m_{ij} x^i y^j = m_{13} x y^3 + m_{22} x^2 y^2 + m_{23} x^2 y^3 = x y^3 + x^2 y^2 + 2 x^2 y^3;$$

$$CoM(\mathbb{Z}_{p^2q}; x, y) = \sum_{i \leq j} \bar{m}_{ij} x^i y^j = \bar{m}_{13} x y^3 + \bar{m}_{22} x^2 y^2 + \bar{m}_{23} x^2 y^3 = 0.$$

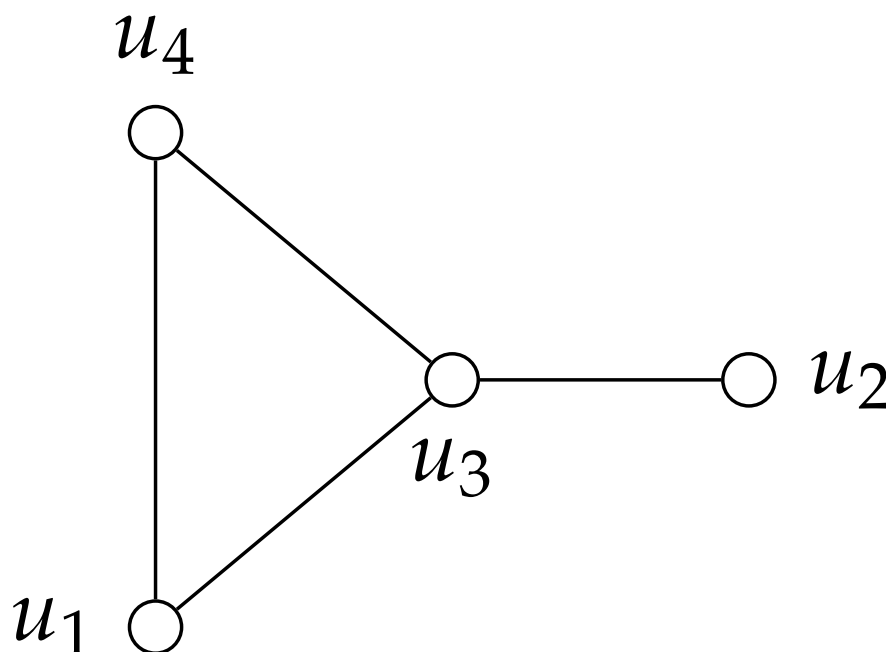


Figure 2. Prime ideal sum graph of \mathbb{Z}_{p^2q} .

In Figure 3, we give the 3D–surface representations of the M -polynomial and CoM -polynomial forms of $PIS(G(\mathbb{Z}_n))$, respectively. \square

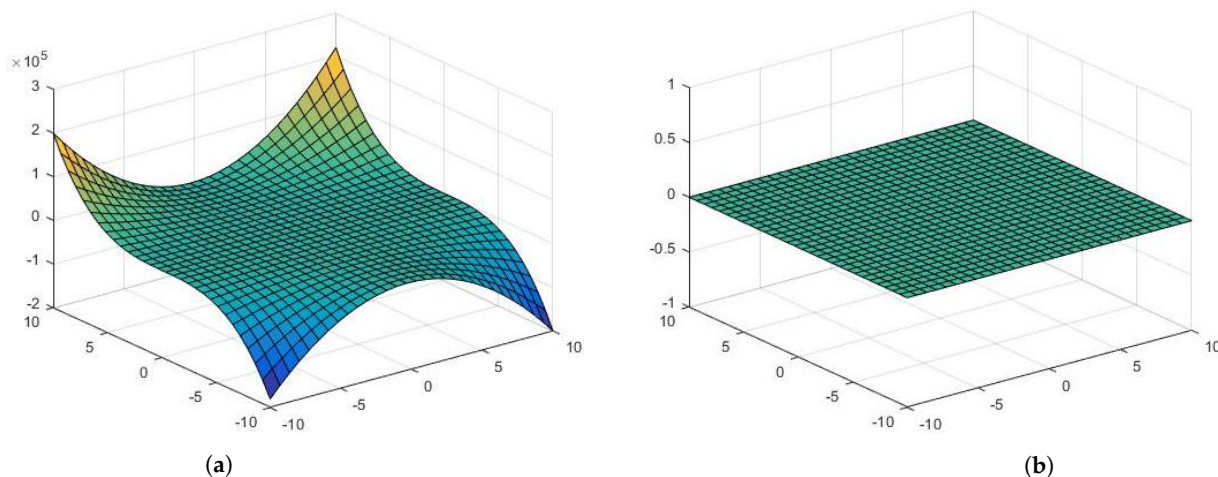


Figure 3. Polynomials corresponding to $PIS(G(\mathbb{Z}_n))$. (a) 3D–surf. of $M(\mathbb{Z}_{p^2q^2}; x, y)$; (b) 3D–surf. of $CoM(\mathbb{Z}_{p^2q^2}; x, y)$.

Theorem 3. Let p and q be distinct prime integers. Then, the M -polynomial and CoM -polynomial of $\mathbb{Z}_{p^2q^2}$ have the forms

$$M(\mathbb{Z}_{p^2q^2}; x, y) = 2x^3y^3 + 8x^3y^4 + 2x^4y^4,$$

$$CoM(\mathbb{Z}_{p^2q^2}; x, y) = 4x^3y^3 + 4x^3y^4 + x^4y^4.$$

Proof. Let us consider the ideals

$$u_1 = p\mathbb{Z}_n, u_2 = q\mathbb{Z}_n, u_3 = pq\mathbb{Z}_n, u_4 = p^2q\mathbb{Z}_n, u_5 = pq^2\mathbb{Z}_n, u_6 = p^2\mathbb{Z}_n, u_7 = q^2\mathbb{Z}_n$$

where u_1 and u_2 are the prime ones and for $n = p^2q^2$. Then, $PIS(\mathbb{Z}_{p^2q^2})$ is as follows:

It can be seen from the PIS -graph structure of $\mathbb{Z}_{p^2q^2}$ in Figure 4 that $d(u_1) = 4$, $d(u_2) = 4$, $d(u_3) = 4$, $d(u_4) = 3$, $d(u_5) = 3$, $d(u_6) = 3$, $d(u_7) = 3$. We obtain $n_3 = 4$, $n_4 = 3$ by the vertex and edge-partition technique. It follows from Lemma 1 that:

$$m_{33} = 2, \quad \bar{m}_{33} = \frac{4 \times 3}{2} - 2 = 4,$$

$$m_{34} = 8, \quad \bar{m}_{33} = 4 \times 3 - 8 = 4,$$

$$m_{44} = 2, \quad \bar{m}_{44} = \frac{3 \times 2}{2} - 2 = 1.$$

Hence, $M(\mathbb{Z}_{p^2q^2}; x, y) = \sum_{i \leq j} m_{ij}x^i y^j = 2x^3y^3 + 8x^3y^4 + 2x^4y^4$ and $CoM(\mathbb{Z}_{p^2q^2}; x, y) = \sum_{i \leq j} \bar{m}_{ij}x^i y^j = 4x^3y^3 + 4x^3y^4 + x^4y^4$ are obtained.

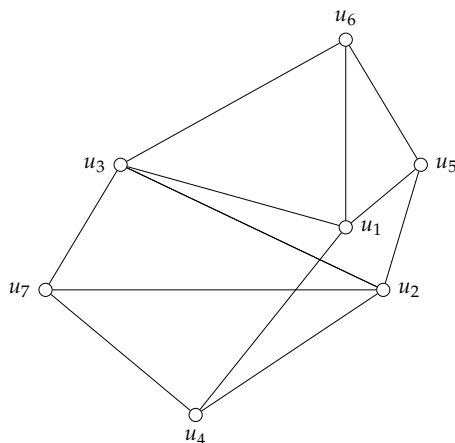


Figure 4. Prime ideal sum graph of $\mathbb{Z}_{p^2q^2}$.

In Figure 5, we give the 3D–surface representations of the M -polynomial and CoM -polynomial forms of $PIS(G(\mathbb{Z}_n))$, respectively. \square

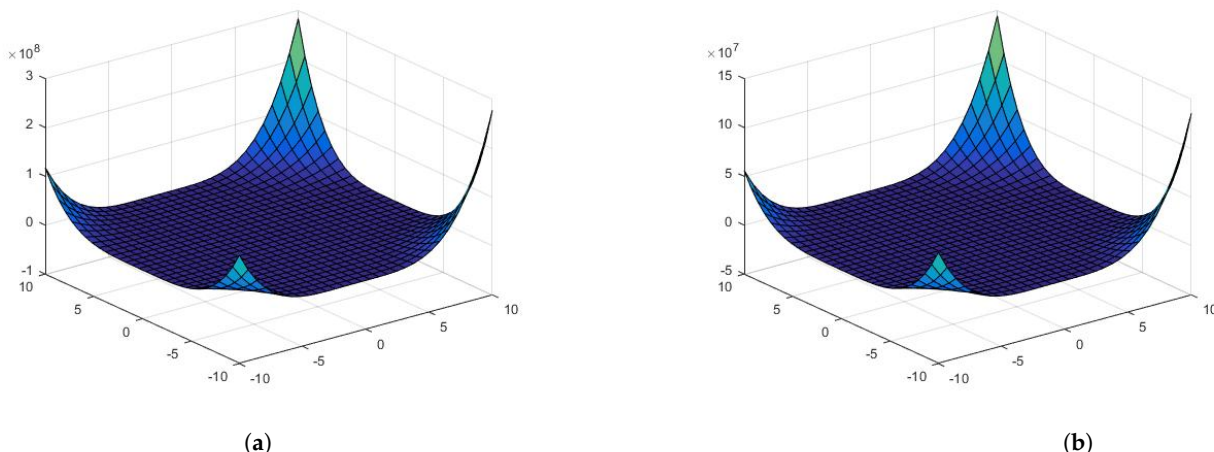


Figure 5. Polynomials corresponding to $PIS(G(\mathbb{Z}_n))$. **(a)** 3D–surf. of $M(\mathbb{Z}_{p^2q^2}; x, y)$; **(b)** 3D–surf. of $CoM(\mathbb{Z}_{p^2q^2}; x, y)$.

Theorem 4. Let $p, q,$ and r be distinct prime integers. Then, the M -polynomial and CoM -polynomial of \mathbb{Z}_{pqr} have the forms

$$M(\mathbb{Z}_{pqr}; x, y) = 6x^2y^4 + 3x^4y^4$$

$$CoM(\mathbb{Z}_{pqr}; x, y) = 3x^2y^4.$$

Proof. Let us consider the ideals $u_1 = p\mathbb{Z}_n, u_2 = q\mathbb{Z}_n, u_3 = r\mathbb{Z}_n, u_4 = pq\mathbb{Z}_n, u_5 = pr\mathbb{Z}_n, u_6 = qr\mathbb{Z}_n,$ where $u_1, u_2,$ and u_3 are the prime ones and $n = pqr.$ Then, $PIS(\mathbb{Z}_{pqr})$ is as follows (see Figure 6):

Taking into account the graph structure of $\mathbb{Z}_{pqr},$ it is obtained that $d(u_1) = 2, d(u_2) = 2, d(u_3) = 2, d(u_4) = 4, d(u_5) = 4, d(u_6) = 4.$ It follows that $n_2 = 3, n_4 = 3$ by vertex partition. Then, we have

$$m_{24} = 6, \quad \bar{m}_{24} = 3 \times 3 - 6 = 3,$$

$$m_{44} = 3, \quad \bar{m}_{44} = \frac{3 \times 2}{2} - 3 = 0$$

by the edge-partition technique. Hence, we obtain:

$$M(\mathbb{Z}_{pqr}; x, y) = \sum_{i \leq j} m_{ij} x^i y^j = 6x^2y^4 + 3x^4y^4,$$

$$CoM(\mathbb{Z}_{pqr}; x, y) = \sum_{i \leq j} \bar{m}_{ij} x^i y^j = 3x^2y^4.$$

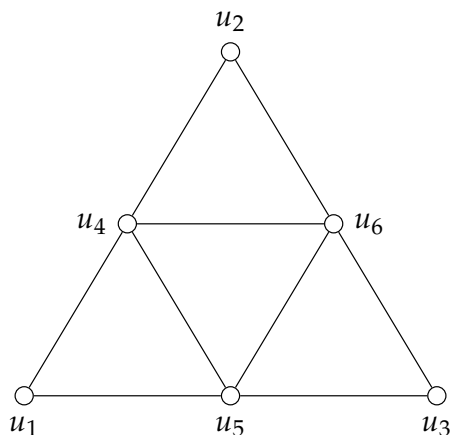


Figure 6. Prime ideal sum graph of $\mathbb{Z}_{pqr}.$

In Figure 7, we give the 3D–surface representations of the M -polynomial and CoM -polynomial forms of $PIS(G(\mathbb{Z}_n)),$ respectively. \square

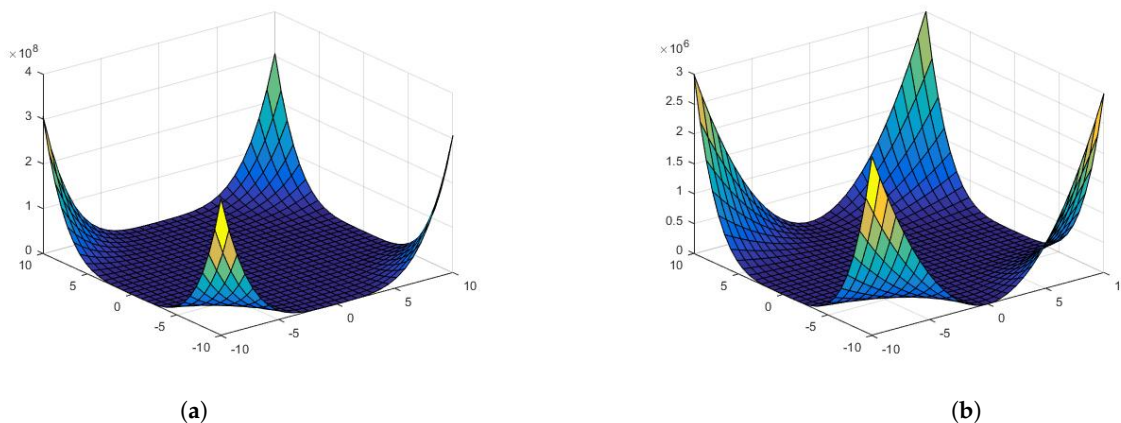


Figure 7. Polynomials corresponding to $PIS(G(\mathbb{Z}_n))$. (a) 3D–surf. of $M(\mathbb{Z}_{pqr}; x, y)$; (b) 3D–surf. of $CoM(\mathbb{Z}_{pqr}; x, y)$.

Theorem 5. Let p and q be distinct prime integers. Then, the M -polynomial and CoM -polynomial of \mathbb{Z}_{p^3q} have the forms

$$M(\mathbb{Z}_{p^3q}; x, y) = x^2y^2 + 6x^2y^4 + x^4y^4,$$

$$CoM(\mathbb{Z}_{p^3q}; x, y) = 5x^2y^2 + 6x^2y^4.$$

Proof. Let us consider the ideals

$$u_1 = p\mathbb{Z}_n, u_2 = q\mathbb{Z}_n, u_3 = p^2\mathbb{Z}_n, u_4 = pq\mathbb{Z}_n, u_5 = p^3\mathbb{Z}_n, u_6 = p^2q\mathbb{Z}_n$$

where u_1 and u_2 are the prime ones for $n = p^3q$. Then, $PIS(\mathbb{Z}_{p^3q})$ is as follows (see Figure 8):

According to the PIS graph of \mathbb{Z}_{p^3q} it is clear that $d(u_1) = 4, d(u_2) = 2, d(u_3) = 2, d(u_4) = 4, d(u_5) = 2, d(u_6) = 2$. It follows that $n_2 = 4$ and $n_4 = 2$ by vertex partition. Thus, the necessary coefficients to construct related polynomials are obtained as follows by edge partition:

$$m_{22} = 2, \quad \bar{m}_{22} = \frac{4 \times 3}{2} - 1 = 5,$$

$$m_{24} = 8, \quad \bar{m}_{24} = 4 \times 2 - 6 = 6,$$

$$m_{44} = 2, \quad \bar{m}_{44} = \frac{2 \times 1}{2} - 1 = 0.$$

Hence, we obtain $M(\mathbb{Z}_{p^3q}; x, y) = \sum_{i \leq j} m_{ij} x^i y^j = x^2y^2 + 6x^2y^4 + x^4y^4$ and $CoM(\mathbb{Z}_{p^3q}; x, y) = \sum_{i \leq j} \bar{m}_{ij} x^i y^j = 5x^2y^2 + 6x^2y^4$.

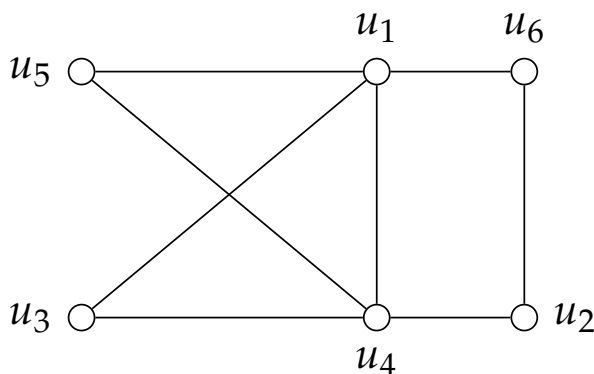


Figure 8. Prime ideal sum graph of \mathbb{Z}_{p^3q} .

In Figure 9, we give the 3D–surface representations of the M -polynomial and CoM -polynomial forms of $PIS(G(\mathbb{Z}_n))$, respectively. \square

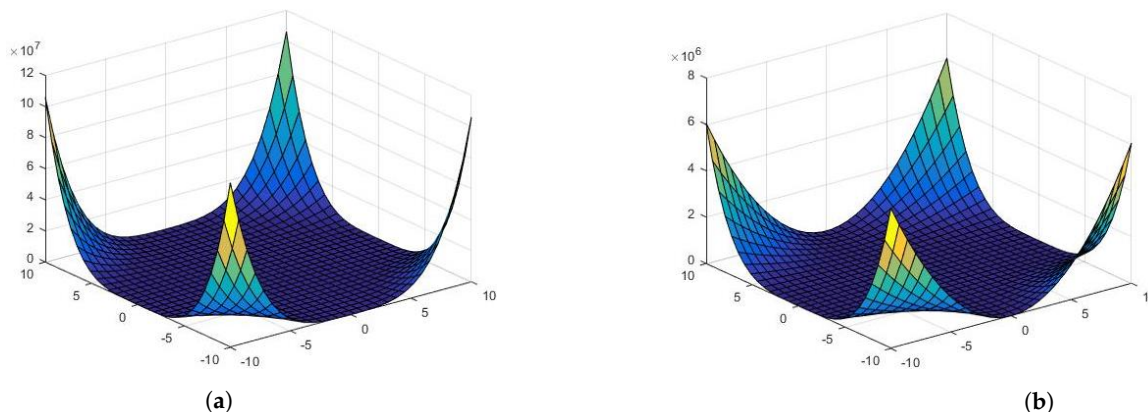


Figure 9. Polynomials corresponding to $PIS(G(\mathbb{Z}_n))$. (a) 3D–surf. of $M(\mathbb{Z}_{p^3q}; x, y)$; (b) 3D–surf. of $CoM(\mathbb{Z}_{p^3q}; x, y)$.

Theorem 6. Let $p, q,$ and r be distinct prime integers. Then, the M -polynomial and CoM -polynomial of \mathbb{Z}_{p^2qr} have the forms

$$M(\mathbb{Z}_{p^2qr}; x, y) = 5x^4y^4 + 14x^4y^6 + 5x^6y^6,$$

$$CoM(\mathbb{Z}_{p^2qr}; x, y) = 16x^4y^4 + 7x^4y^6 - 2x^6y^6.$$

Proof. Let us consider the ideals $u_1 = p\mathbb{Z}_n, u_2 = q\mathbb{Z}_n, u_3 = r\mathbb{Z}_n, u_4 = p^2\mathbb{Z}_n, u_5 = pq\mathbb{Z}_n, u_6 = pr\mathbb{Z}_n, u_7 = p^2q\mathbb{Z}_n, u_8 = p^2r\mathbb{Z}_n, u_9 = qr\mathbb{Z}_n, u_{10} = pqr\mathbb{Z}_n$, where $u_1, u_2,$ and u_3 are the prime ones and $n = p^2qr$. Then, $PIS(\mathbb{Z}_{p^2qr})$ is as follows (see Figure 10):

It can be seen from the PIS -graph structure of \mathbb{Z}_{p^2qr} that $d(u_1) = 6, d(u_2) = 4, d(u_3) = 4, d(u_4) = 4, d(u_5) = 6, d(u_6) = 6, d(u_7) = 4, d(u_8) = 4, d(u_9) = 6, d(u_{10}) = 4$. Here, we obtain $n_4 = 6, n_6 = 4$ using the vertex partition technique. In addition, we obtain from Lemma 1 that:

$$m_{44} = 5, \quad \bar{m}_{44} = \frac{7 \times 6}{2} - 5 = 16$$

$$m_{46} = 14, \quad \bar{m}_{46} = 7 \times 3 - 14 = 7$$

$$m_{66} = 5, \quad \bar{m}_{66} = \frac{3 \times 2}{2} - 5 = -2$$

by the edge-partition technique.

Hence, $M(\mathbb{Z}_{p^2qr}; x, y) = \sum_{i \leq j} m_{ij}x^i y^j = 5x^4y^4 + 14x^4y^6 + 5x^6y^6$ and $CoM(\mathbb{Z}_{p^2qr}; x, y) = \sum_{i \leq j} \bar{m}_{ij}x^i y^j = 16x^4y^4 + 7x^4y^6 - 2x^6y^6$ are obtained.

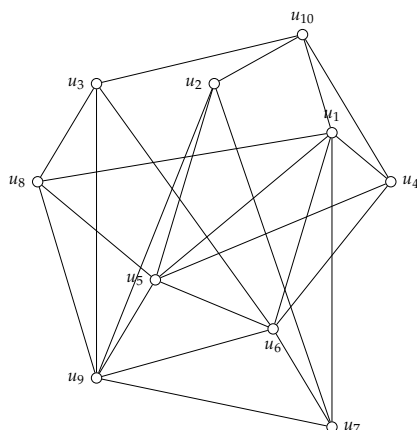


Figure 10. Prime ideal sum graph of \mathbb{Z}_{p^2qr} .

In Figure 11, we give the 3D–surface representations of the M -polynomial and CoM -polynomial forms of $PIS(G(\mathbb{Z}_n))$, respectively. \square

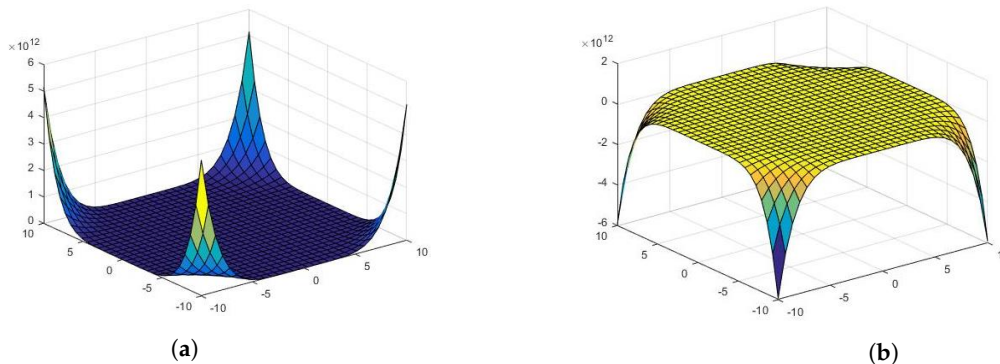


Figure 11. Polynomials corresponding to $PIS(G(\mathbb{Z}_n))$. (a) 3D–surf. of $M(\mathbb{Z}_{p^2qr}; x, y)$; (b) 3D–surf. of $CoM(\mathbb{Z}_{p^2qr}; x, y)$.

Theorem 7. Let $p, q, r,$ and s be distinct prime integers. Then, the M -polynomial and CoM -polynomial of \mathbb{Z}_{pqrs} have the forms

$$M(\mathbb{Z}_{pqrs}; x, y) = 11x^6y^6 + 25x^6y^8 + 12x^8y^8,$$

$$CoM(\mathbb{Z}_{pqrs}; x, y) = 17x^6y^6 + 23x^6y^8 + 3x^8y^8.$$

Proof. Let us consider the ideals $u_1 = p\mathbb{Z}_n, u_2 = q\mathbb{Z}_n, u_3 = r\mathbb{Z}_n, u_4 = pq\mathbb{Z}_n, u_5 = s\mathbb{Z}_n, u_6 = pr\mathbb{Z}_n, u_7 = ps\mathbb{Z}_n, u_8 = qr\mathbb{Z}_n, u_9 = qs\mathbb{Z}_n, u_{10} = pqr\mathbb{Z}_n, u_{11} = rs\mathbb{Z}_n, u_{12} = pqs\mathbb{Z}_n, u_{13} = prs\mathbb{Z}_n, u_{14} = qrs\mathbb{Z}_n$ where $u_1, u_2, u_3,$ and u_5 are the prime ones and $n = pqrs$. Then, $PIS(\mathbb{Z}_{pqrs})$ is given in Figure 12.

From the PIS -graph structure of \mathbb{Z}_{pqrs} , we have $d(u_1) = d(u_2) = d(u_3) = d(u_5) = d(u_{10}) = d(u_{12}) = d(u_{13}) = d(u_{14}) = 6$ and $d(u_4) = d(u_6) = d(u_7) = d(u_8) = d(u_9) = d(u_{11}) = 8$. Using the vertex partition technique, we have $n_6 = 8$ and $n_8 = 6$. By edge partition and using Lemma 1, we obtain:

$$m_{66} = 11, \quad \bar{m}_{66} = \frac{8 \times 7}{2} - 11 = 17,$$

$$m_{68} = 25, \quad \bar{m}_{68} = 8 \times 6 - 25 = 23,$$

$$m_{88} = 12, \quad \bar{m}_{88} = \frac{6 \times 5}{2} - 12 = 3.$$

Hence, $M(\mathbb{Z}_{pqrs}; x, y) = 11x^6y^6 + 25x^6y^8 + 12x^8y^8$, and $CoM(\mathbb{Z}_{pqrs}; x, y) = 17x^6y^6 + 23x^6y^8 + 3x^8y^8$ are obtained.

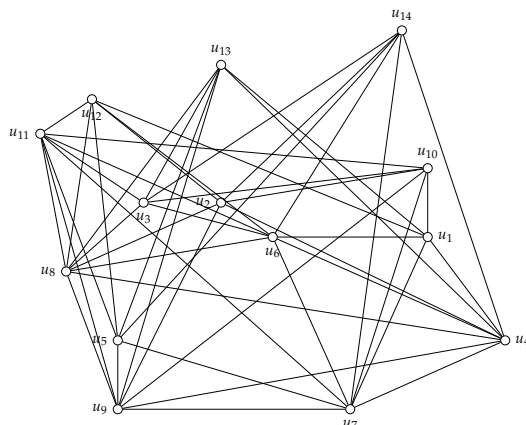


Figure 12. Prime ideal sum graph of \mathbb{Z}_{pqrs} .

In Figure 13, we give the 3D–surface representations of the M -polynomial and CoM -polynomial forms of $PIS(G(\mathbb{Z}_n))$, respectively. \square

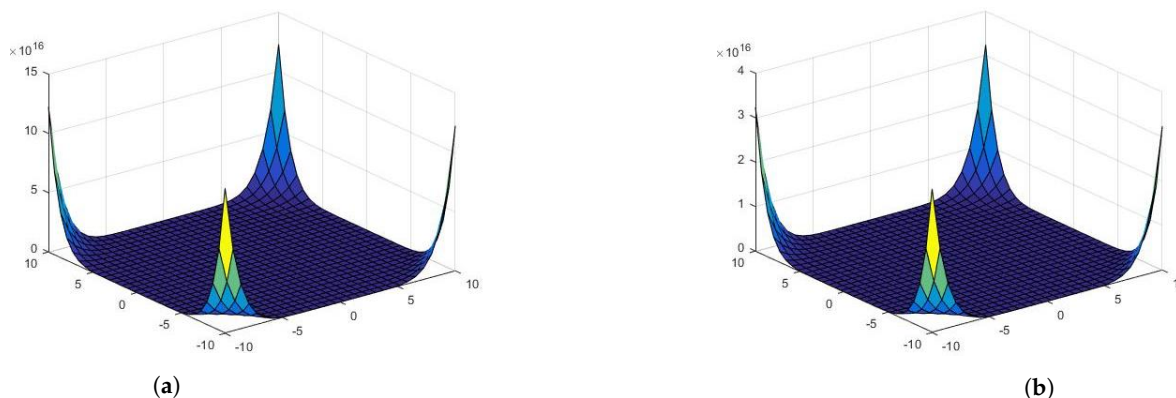


Figure 13. Polynomials corresponding to $PIS(G(\mathbb{Z}_n))$. (a) 3D–surf. of $M(\mathbb{Z}_{pqrs}; x, y)$; (b) 3D–surf. of $CoM(\mathbb{Z}_{pqrs}; x, y)$.

5.2. Computing Various Topological Indices and Topological Coindices of Some Commutative Rings

Since the proofs of the theorems in this section are similar to each other, only a few of them are discussed. The others can be proven by the same technique with necessary variations via the related M -polynomials and CoM -polynomials of \mathbb{Z}_n .

5.2.1. Topological Indices

Theorem 8. Let G be the PIS graph of \mathbb{Z}_p^α for $\alpha \geq 2$. Then,

$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
$\alpha^2 - 3\alpha + 2$	$(\alpha - 2)^2$	1	$\alpha^3 - 5\alpha^2 + 8\alpha - 4$	$\alpha^3 - 6\alpha^2 + 10\alpha - 4$	$\alpha^2 - 4\alpha + 5$	$\frac{2\alpha - 4}{\alpha - 1}$	$\frac{(\alpha - 2)^2}{\alpha - 1}$	$\frac{(\alpha - 2)^4}{(\alpha - 3)^3}$

Proof. Since $M(\mathbb{Z}_p^\alpha; x, y) = (\alpha - 2)xy^{\alpha-2}$ and $\alpha \geq 2$ from Theorem 1, we have the following results from Table 1.

$$\begin{aligned}
 D_x &= (\alpha - 2)xy^{\alpha-2}, & D_y &= (\alpha - 2)^2xy^{\alpha-2} \\
 S_x &= (\alpha - 2)xy^{\alpha-2}, & S_y &= xy^{\alpha-2}, \\
 D_x + D_y &= (\alpha^2 - 3\alpha + 2)xy^{\alpha-2}, \\
 D_x D_y &= (\alpha - 2)^2xy^{\alpha-2}, \\
 S_x S_y &= xy^{\alpha-2}, \\
 D_x D_y (D_x + D_y) &= (\alpha^3 - 5\alpha^2 + 8\alpha - 4)xy^{\alpha-2}, \\
 D_x^2 &= (\alpha - 2)xy^{\alpha-2}, & D_y^2 &= (\alpha - 2)^3xy^{\alpha-2}, \\
 D_x^2 + D_y^2 &= (\alpha^3 - 6\alpha^2 + 10\alpha - 4)xy^{\alpha-2}, \\
 D_x S_y + S_x D_y &= (\alpha^2 - 4\alpha + 5)xy^{\alpha-2}, \\
 2S_x J &= \frac{2\alpha - 4}{\alpha - 1}x^{\alpha-1}, \\
 S_x J D_x D_y &= \frac{(\alpha - 2)^2}{\alpha - 1}x^{\alpha-1}, \\
 S_x^3 Q_{-2} J D_x^3 D_y^3 &= \frac{(\alpha - 2)^4}{(\alpha - 3)^3}x^{\alpha-3}.
 \end{aligned}$$

Hence, we obtain $M_1 = (\alpha^2 - 3\alpha + 2)$, $M_2 = (\alpha - 2)^2$, $mM_2 = 1$, $RezG_3 = \alpha^3 - 5\alpha^2 + 8\alpha - 4$, $F = \alpha^3 - 6\alpha^2 + 10\alpha - 4$, $SDD = (\alpha^2 - 4\alpha + 5)$, $H = \frac{2\alpha - 4}{\alpha - 1}$, $I = \frac{(\alpha - 2)^2}{\alpha - 1}$, and $A = \frac{(\alpha - 2)^4}{(\alpha - 3)^3}$ for $x = y = 1$. \square

Theorem 9. Let G be the PIS graph of \mathbb{Z}_{p^2q} . Then,

$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
18	19	0.916	88	32	21.666	1.8	4.15	4.877

Proof. Taking into account $M(\mathbb{Z}_{p^2q}; x, y) = xy^3 + x^2y^2 + 2x^2y^3$ from Theorem 2, we have the following results.

$$\begin{aligned}
 D_x &= xy^3 + 2x^2y^2 + 4x^2y^3, D_y = 3xy^3 + 2x^2y^2 + 6x^2y^3 \\
 S_x &= xy^3 + \frac{1}{2}x^2y^2 + x^2y^3, S_y = \frac{1}{3}xy^3 + \frac{1}{2}x^2y^2 + \frac{2}{3}x^2y^3, \\
 D_x + D_y &= 4xy^3 + 4x^2y^2 + 10x^2y^3, \\
 D_x D_y &= 3xy^3 + 4x^2y^2 + 12x^2y^3, \\
 S_x S_y &= \frac{1}{3}xy^3 + \frac{1}{4}x^2y^2 + \frac{1}{3}x^2y^3, \\
 D_x D_y (D_x + D_y) &= 12xy^3 + 16x^2y^2 + 60x^2y^3, \\
 D_x^2 &= xy^3 + 4x^2y^2 + 8x^2y^3, D_y^2 = 3xy^3 + 4x^2y^2 + 12x^2y^3, \\
 D_x^2 + D_y^2 &= 4xy^3 + 8x^2y^2 + 20x^2y^3, \\
 D_x S_y + S_x D_y &= \frac{10}{3}xy^3 + 5x^2y^2 + \frac{40}{3}x^2y^3, \\
 2S_x I &= x^4 + \frac{4}{5}x^5, \\
 S_x J D_x D_y &= \frac{7}{4}x^4 + \frac{12}{5}x^5, \\
 S_x^3 Q_{-2} J D_x^3 D_y^3 &= \frac{91}{64}x^4 + \frac{432}{125}x^5.
 \end{aligned}$$

Hence, we obtain from Table 1 $M_1 = 18, M_2 = 19, mM_2 = 0.916, RezG_3 = 88, F = 32, SDD = 21.666, H = 1.8, I = 4.15,$ and $A = 4.877.$ □

The proofs of Theorems 10–14 are similar to the proof of Theorem 9.

Theorem 10. Let G be the PIS graph of $\mathbb{Z}_{p^2q^2}$. Then,

$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
84	146	0.626	1036	300	24.666	3.452	20.714	159.909

Theorem 11. Let G be the PIS graph of \mathbb{Z}_{pqr} . Then,

$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
60	96	0.937	480	168	21	2.75	14	104.888

Theorem 12. Let G be the PIS graph of \mathbb{Z}_{p^3q} . Then,

$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
48	68	1.062	432	160	19	2.75	11	17.240

Theorem 13. Let G be the PIS graph of \mathbb{Z}_{p^2qr} . Then,

$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
240	596	1.034	6160	1248	50.333	4.883	58.6	706.094

Theorem 14. Let G be the PIS graph of \mathbb{Z}_{pqrs} . Then,

$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
674	2364	1.013	33,840	4824	98.083	6.904	166.714	3259.618

5.2.2. Topological Coindices

Theorem 15. Let G be the PIS graph of \mathbb{Z}_{p^α} for $\alpha \geq 2$. Then,

$\overline{M}_1(G)$	$\overline{M}_2(G)$	$\overline{mM}_2(G)$	$\overline{RezG}_3(G)$	$\overline{F}(G)$	$\overline{SDD}(G)$	$\overline{H}(G)$	$\overline{I}(G)$	$\overline{A}(G)$
0	0	0	0	0	0	0	0	0

Proof. Since $CoM(\mathbb{Z}_{p^\alpha}; x, y) = 0$, then it is a clear fact that all coindices are equal to zero. □

Theorem 16. Let G be the PIS graph of \mathbb{Z}_{p^2q} . Then,

$\overline{M}_1(G)$	$\overline{M}_2(G)$	$\overline{mM}_2(G)$	$\overline{RezG}_3(G)$	$\overline{F}(G)$	$\overline{SDD}(G)$	$\overline{H}(G)$	$\overline{I}(G)$	$\overline{A}(G)$
0	0	0	0	0	0	0	0	0

Proof. Since $CoM(\mathbb{Z}_{p^2q}; x, y) = 0$, then it is a clear fact that all coindices are equal to zero. □

Theorem 17. Let G be the PIS graph of $\mathbb{Z}_{p^2q^2}$. Then,

$\overline{M}_1(G)$	$\overline{M}_2(G)$	$\overline{mM}_2(G)$	$\overline{RezG}_3(G)$	$\overline{F}(G)$	$\overline{SDD}(G)$	$\overline{H}(G)$	$\overline{I}(G)$	$\overline{A}(G)$
60	100	0.840	377	204	18.333	2.726	14.857	119.821

Proof. Taking into account the form of the CoM-polynomial $CoM(\mathbb{Z}_{p^2q^2}; x, y) = 4x^3y^3 + 4x^3y^4 + x^4y^4$ from Theorem 3, we have the following results.

$$\begin{aligned}
 D_x &= 12x^3y^3 + 12x^3y^4 + 4x^4y^4, D_y = 12x^3y^3 + 16x^3y^4 + 4x^4y^4 \\
 S_x &= \frac{4}{3}x^3y^3 + \frac{4}{3}x^3y^4 + \frac{1}{4}x^4y^4, S_y = \frac{4}{3}x^3y^3 + x^3y^4 + \frac{1}{4}x^4y^4, \\
 D_x + D_y &= 24x^3y^3 + 28x^3y^4 + 8x^4y^4, \\
 D_x D_y &= 36x^3y^3 + 48x^3y^4 + 16x^4y^4, \\
 S_x S_y &= \frac{4}{9}x^3y^3 + \frac{1}{3}x^3y^4 + \frac{1}{16}x^4y^4, \\
 D_x D_y (D_x + D_y) &= 216x^3y^3 + 336x^3y^4 + 128x^4y^4, \\
 D_x^2 &= 36x^3y^3 + 36x^3y^4 + 16x^4y^4, D_y^2 = 36x^3y^3 + 64x^3y^4 + 16x^4y^4, \\
 D_x^2 + D_y^2 &= 72x^3y^3 + 100x^3y^4 + 32x^4y^4, \\
 D_x S_y + S_x D_y &= 8x^3y^3 + \frac{25}{3}x^3y^4 + 2x^4y^4, \\
 2S_x J &= \frac{4}{3}x^6 + \frac{8}{7}x^7 + \frac{1}{4}x^8, \\
 S_x J D_x D_y &= 6x^6 + \frac{48}{7}x^7 + 2x^8, \\
 S_x^3 Q_{-2} J D_x^3 D_y^3 &= \frac{2916}{64}x^6 + \frac{6912}{125}x^7 + \frac{4096}{216}x^8.
 \end{aligned}$$

Hence, we obtain from Table 2 that $\overline{M}_1 = 60$, $\overline{M}_2 = 100$, $\overline{mM}_2 = 0.840$, $\overline{RezG}_3 = 377$, $\overline{F} = 204$, $\overline{SDD} = 18.333$, $\overline{H} = 2.726$, $\overline{I} = 14.857$, and $\overline{A} = 119.821$. \square

The proofs of Theorems 18–21 are similar to the proof of Theorem 17.

Theorem 18. The topological coindices of PIS graph $G(\mathbb{Z}_{pqr})$ are computed as follows:

$\overline{M}_1(G)$	$\overline{M}_2(G)$	$\overline{mM}_2(G)$	$\overline{RezG}_3(G)$	$\overline{F}(G)$	$\overline{SDD}(G)$	$\overline{H}(G)$	$\overline{I}(G)$	$\overline{A}(G)$
18	24	0.375	144	60	7.5	1	4	24

Theorem 19. The topological coindices of PIS graph $G(\mathbb{Z}_{p^3q})$ are computed as follows:

$\overline{M}_1(G)$	$\overline{M}_2(G)$	$\overline{mM}_2(G)$	$\overline{RezG}_3(G)$	$\overline{F}(G)$	$\overline{SDD}(G)$	$\overline{H}(G)$	$\overline{I}(G)$	$\overline{A}(G)$
56	68	2	368	160	25	4.5	13	88

Theorem 20. The topological coindices of PIS graph $G(\mathbb{Z}_{p^2qr})$ are computed as follows:

$\overline{M}_1(G)$	$\overline{M}_2(G)$	$\overline{mM}_2(G)$	$\overline{RezG}_3(G)$	$\overline{F}(G)$	$\overline{SDD}(G)$	$\overline{H}(G)$	$\overline{I}(G)$	$\overline{A}(G)$
174	224	0.986	2864	732	43.166	5.066	−6.8	399.095

Theorem 21. The topological coindices of PIS graph $G(\mathbb{Z}_{pqrs})$ are computed as follows:

$\overline{M}_1(G)$	$\overline{M}_2(G)$	$\overline{mM}_2(G)$	$\overline{RezG}_3(G)$	$\overline{F}(G)$	$\overline{SDD}(G)$	$\overline{H}(G)$	$\overline{I}(G)$	$\overline{A}(G)$
674	2364	1.013	33,840	4824	98.083	6.904	166.714	2551.752

5.3. Comparison

In this part of the study, considering each M -polynomial and CoM -polynomial designed for algebraic graph structures studied in previous sections, we give the table (Figure 14) of computed values of topological descriptors in order to shed a visual light on its physical and topological features.

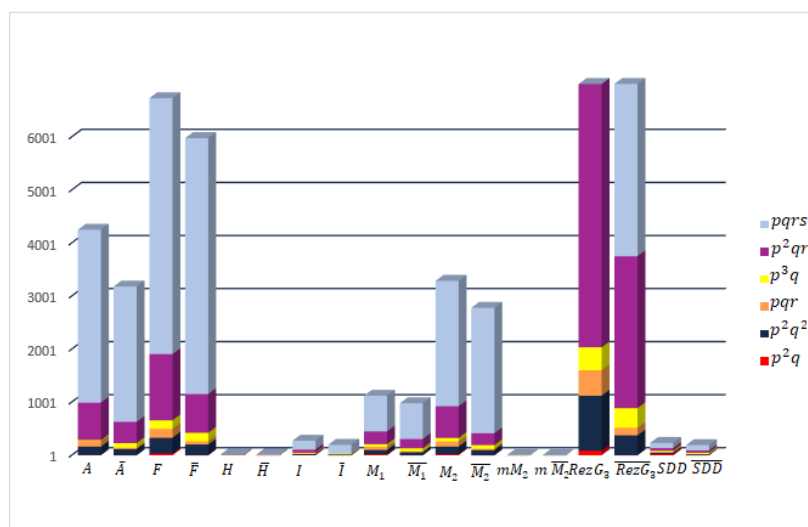


Figure 14. Numerical and graphical comparison of topological indices and coindices.

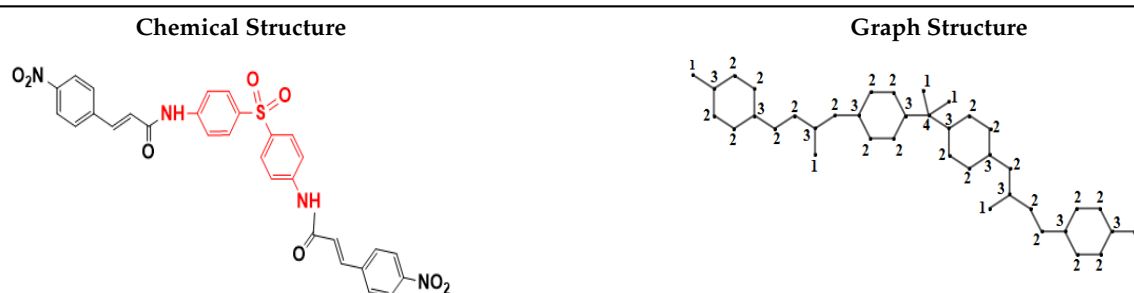
6. Applications in Chemistry

In the present section, we discuss applications of algebraic graph theory in chemistry. We aim to present a chemical application to emphasize the positive impact of degree-based topological (co)indices on QSAR analysis. Our statistical analysis verifies that the study's topological descriptors are good predictors of various bioactivity properties of the seven anti-Alzheimer drug candidates.

Significant contributions have been made in the field of investigating the predictive potential of different classes of graph-theoretic indices. The first study combining topological descriptors with QSAR analysis was carried out in [51]. Another study was undertaken by Gutman and Tošovic [52], who initiated a comprehensive examination to evaluate the efficacy of degree-based topological indices in predicting the physicochemical properties of isomeric octanes. In [53], Malik et al. broadened their research scope, moving beyond isomeric octanes to encompass benzenoid hydrocarbons, in order to establish correlations between various physicochemical properties. Furthermore, Hayat et al. [54] extended their study to lower polycyclic aromatic hydrocarbons for correlating the π -electron energy. Hayat and Asmat [55] discovered the optimal value of α that yields the strongest correlation between the generalized first Zagreb index M_1^α and the π -electron energy of lower benzenoid hydrocarbons. Arif et al. [56] explored the predictive capacity of degree-based irregularity indices concerning the physicochemical characteristics of monocarboxylic acids. In [57,58], the authors expanded upon previous research, investigating the predictive potential of topological indices, shifting the focus from degree-based indices to distance-based indices. References [59–63] can also be cited for eigenvalues-based indices and their ability to predict various properties. In this part of the study, we harnessed QSAR modeling to perform an elaborate regression analysis, showcasing its predictive power in relation to our degree-based topological descriptors.

With this aim, we chose seven compounds (Compound 1, Compound 2, Compound 3, Compound I, Compound III, Compound IV, and Compound VI) that were claimed as effective Alzheimer's disease drug candidates by testing limited experimental methods in [64,65]. Now, we will explain in detail, for one of the compounds (Compound 3), that the calculations we made for algebraic graphs are similar for chemical graphs. Let $G = (V(G), E(G))$ be the chemical graph of Compound 3 taken from [64]. The compound's molecular graph contains 39 vertices and 41 edges as follows (see Table 3 below):

Table 3. Graph representation of molecular structure.



$$V_1 = \{u \in V(G) : d(u) = 1\}, n_1 = |V_1| = 6; V_2 = \{u \in V(G) : d(u) = 2\}, n_2 = |V_2| = 22 \\ V_3 = \{u \in V(G) : d(u) = 3\}, n_3 = |V_3| = 10; V_4 = \{u \in V(G) : d(u) = 4\}, n_4 = |V_4| = 1$$

Since the vertex partition of the chemical compound is as above, we have $n_1 = |V_1| = 6$, $n_2 = |V_2| = 22$, $n_3 = |V_3| = 10$, $n_4 = |V_4| = 1$.

Additionally, if $E_{ij} = \{uv = e_{ij} \in E(G) : d(u) = i \wedge d(v) = j\}$ and $|E_{ij}| = m_{ij}$, then the coefficients of the M -polynomial and also the coefficients of the CoM -polynomial of the chemical compound can be determined as follows using the edge-partition technique.

$$\begin{aligned}
 |E_{13}| &= m_{13} = 4; \bar{m}_{13} = n_1 n_3 - m_{13} = 6 \times 10 - 4 = 56 \\
 |E_{23}| &= m_{23} = 24; \bar{m}_{23} = n_2 n_3 - m_{23} = 22 \times 10 - 24 = 196 \\
 |E_{14}| &= m_{14} = 2; \bar{m}_{22} = n_1 n_4 - m_{14} = 6 \times 1 - 2 = 4 \\
 |E_{22}| &= m_{22} = 9; \bar{m}_{14} = \frac{n_2(n_2 - 1)}{2} - m_{22} = \frac{22(22 - 1)}{2} - 9 = 222 \\
 |E_{34}| &= m_{34} = 2; \bar{m}_{34} = n_3 n_4 - m_{34} = 10 \times 1 - 2 = 8
 \end{aligned}$$

Hence, the polynomials are obtained as follows:

$$\begin{aligned}
 M(x, y) &= \sum_{i \leq j} m_{ij} x^i y^j = 4xy^3 + 2xy^4 + 9x^2y^2 + 24x^2y^3 + 2x^3y^4 \\
 CoM(x, y) &= \sum_{i \leq j} \bar{m}_{ij} x^i y^j = 56xy^3 + 4xy^4 + 222x^2y^2 + 196x^2y^3 + 8x^3y^4.
 \end{aligned}$$

When similar processes are applied to the remaining molecules in order to calculate the topological indices, we obtain the results given in Table 4 below.

Table 4. The values of topological indices calculated with respect to the graph structure of the compounds.

Compounds	$M_1(G)$	$M_2(G)$	$mM_2(G)$	$RezG_3(G)$	$F(G)$	$SDD(G)$	$H(G)$	$I(G)$	$A(G)$
Compound 1	186.00	208.00	8.17	956.00	458.00	89.67	17.4	43.2	301.50
Compound 2	186.00	208.00	8.17	956.00	458.00	89.67	17.4	43.2	301.50
Compound 3	284.00	416.00	8.25	1744.00	716.00	97.33	17.47	81.49	309.89
Compound I	182.00	212.00	7.67	1064.00	466.00	87.00	16.2	43.1	296.59
Compound III	196.00	232.00	8.00	1212.00	408.00	95.33	16.77	45.73	312.98
Compound IV	186.00	210.00	8.22	1182.00	458.00	89.00	17.47	44.4	308.28
Compound VI	200.00	230.00	8.56	1156.00	516.00	97.3	18.04	47.03	650.61

Table 5. pMIC ($\mu\text{g}/\text{mL}$) values of the compounds.

Compound	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>K. pneumoniae</i>	<i>E. faecalis</i>	<i>B. cereus</i>	<i>S. aureus</i>
Compound 1	2.71	3.01	2.71	2.71	2.71	2.71
Compound 2	2.11	2.41	2.41	2.11	2.11	2.11
Compound 3	1.81	2.11	1.81	1.81	1.81	1.81
Compound I	3.01	3.01	3.01	3.01	3.01	3.01
Compound III	2.41	2.41	2.41	2.41	2.41	2.41
Compound IV	2.71	3.01	2.71	2.71	2.71	2.11
Compound VI	2.71	3.01	3.01	2.71	2.71	2.71

The following equations give the mathematical connection between features and topological indices that are well correlated in predicting bioactivity properties (see Table 5), with curvilinear regression analysis in exponential form (obtained by SPSS (21.0.)). The fitted curves summarizing this situation are given in Figure 15. The notations R and SE given in the equations state the correlation coefficient and standard error, respectively.

$$E. coli = 5.29 \times (e^{-0.04 \times M_1}); R = 0.777, SE = 0.122$$

$$P. aeruginosa = 3.81 \times (e^{-0.001 \times M_2}); R = 0.727, SE = 0.112$$

$$K. pneumoniae = 4.12 \times (e^{-0.002 \times M_2}); R = 0.848, SE = 0.102$$

$$E. faecalis = 5.298 \times (e^{-0.004 \times M_1}); R = 0.777, SE = 0.122$$

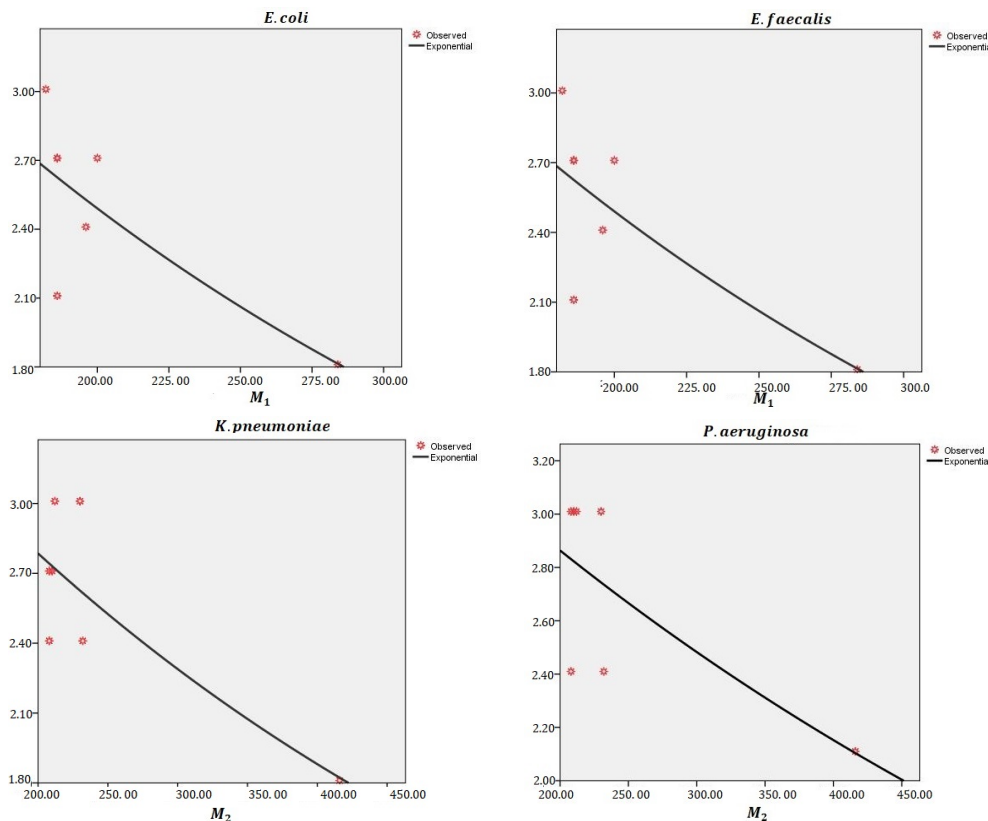


Figure 15. Fitted curves obtained with curvilinear regression analysis in exponential form.

7. Conclusions

Studying algebraic graph theory has high significance in view of combining representation and number theory via combinatoric applications. Applications of finite rings and other fields provide a solid background to cryptology and coding theory. Computing different types of topological indices of algebraic graphs gives an idea about the physical properties of related finite commutative rings. Investigating their different polynomial forms also enables designing new and stronger physical structures in mechanics for robotics. When combining this graph-theoretic-based mathematical modeling with artificial intelligence and mechanic science, it is possible to provide time and budget savings while producing solutions for various computer-network problems. Studying zero-divisor graphs over \mathbb{Z}_n is now a trending field for understanding the physical properties of algebraic structures and is also important for the spectral branch of graph theory.

In this study, we computed some topological indices and coindices that are related to the graph complement of the PIS graph of \mathbb{Z}_n , where $n = p^\alpha, p^2q, p^2q^2, pqr, p^3q$, and $p^2qr, pqrs$ for different prime integers p, q, r , and s , to simplify the process of computing and also obtain an idea of the physical structures of commutative rings. Additionally, we handled some algebraic polynomials called M -polynomials and CoM -polynomials. Both polynomials can be used by researchers in the future, for example, by using QSPR/QSAR analysis in chemistry and in other applied sciences such as cryptology, code theory, and mechanics. Finally, we discussed the applicability of algebraic graphs to chemical graph theory. Studying QSPR/QSAR analysis might be attractive for further studies in the near future. We conclude this section with the following open problem based on the reviewers' comments:

Problem 1. How can we construct the M -polynomials and CoM -polynomials to compute the degree-based topological (co)indices of the PIS graph of \mathbb{Z}_n , where $n = p^\alpha q^\alpha r^\alpha s^\alpha$ for the different prime integers p, q, r, s , and $\alpha \geq 1$?

Author Contributions: Conceptualization, E.Ö.S. and C.A.; methodology, T.A. and S.A.; software, E.Ö.S.; validation, T.A. and S.A.; formal analysis, E.Ö.S.; investigation, E.Ö.S., T.A., C.A. and S.A.; resources, T.A., C.A. and S.A.; data curation, E.Ö.S. and C.A.; writing—review and editing, E.Ö.S. and S.A.; visualization, S.A. and T.A.; supervision, C.A., S.A. and S.A.; project administration, T.A. and S.A. (for the first project); and C.A. and S.A. (for the second project). All authors have read and agreed to the published version of the manuscript.

Funding: This study was carried out with financial support from King Saud University, College of Science, Riyadh, Saudi Arabia under Researchers Supporting Project Number: RSPD2023R934. The work of third and fourth authors was supported by TUBITAK, the Scientific and Technological Research Council of Turkey, under the program “2221-Fellowship for Visiting Professor/Scientists” at Karamanoglu Mehmetbey University (KMU), Turkey.

Data Availability Statement: All data used here is applicable in the article.

Acknowledgments: The authors would like to thank the reviewers for their valuable suggestions and useful comments, which helped us improve the presentation of the manuscript. Moreover, the authors extend their appreciation to King Saud University, the College of Science for funding this research and gratefully acknowledge the TUBITAK for technical and financial support.

Conflicts of Interest: The authors declare no conflict of interest.

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