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Reformulated Zagreb Indices of Some Cycle-Related Graphs and Linear [n]-Phenylenes

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ABSTRACT

Graph invariants (topological indices) are numerical values of graphs obtained from 2-dimensional (2-D) images of chemical structures. These invariants are used in the structure-property/activity studies to predict certain properties such as the enthalpy of vaporization, and stability of molecular structures. In this paper, reformulated Zagreb indices, which are edge-degree-based indices, are considered. First, the reformulated Zagreb indices for cycle-related graphs which are wheel, helm, gear, friendship, closed helm, flower, sun, and sunflower are computed. The values of the first and second reformulated Zagreb indices of cycle-related these graphs and also the values of reformulated Zagreb indices of graphs with the same edge cardinality among studied graphs are compared numerically with the MATLAB software program. Finally, reformulated first Zagreb index and reformulated second Zagreb index of linear [n]-phenylenes are calculated and these values are computed numerically.

Devir İçeren Bazı Grafların ve Lineer [n]-Phenylenlerin Yeniden Formüle Edilmiş Zagreb İndeksleri

Araştırma Makalesi

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Anahtar Kelimeler:
Kimyasal graf teori
Topolojiksel indeks
Devir içeren graflar
Yeniden formüle edilmiş Zagreb indeksleri
Lineer [n]-phenylenler

ÖZ

Graf değişmezleri (topolojik indeksler), kimyasal yapıların 2 boyutlu görüntülerinden elde edilen grafların sayısal değerleridir. Bu değişmezler, moleküler yapıların buharlaşma entalpisi ve kararlılığı gibi belirli özellikleri tahmin etmek için yapı-özellik/aktivite çalışmalarında kullanılır. Bu çalışmada kenar derece tabanlı indekslerden yeniden formüle edilmiş Zagreb indeksleri ele alınmıştır. İlk olarak, tekerlek, dümen, dişli, arkadaşlık, kapalı dümen, çiçek, güneş ve ayçiçeği gibi devir içeren graflar için yeniden formüle edilmiş Zagreb indeksleri hesaplanır. Son olarak, devir içeren bu grafların birinci ve ikinci yeniden formüle edilmiş Zagreb indekslerinin değerleri ve ayrıca çalışılan graflar arasında aynı kenar kardinalitesine sahip grafların yeniden formüle edilmiş Zagreb indekslerinin değerleri MATLAB yazılım programı ile sayısal olarak karşılaştırılmıştır. Son olarak, doğrusal [n]-fenilenlerin yeniden formüle edilmiş birinci Zagreb indeksi ve yeniden formüle edilmiş ikinci Zagreb indeksi hesaplanmış ve bu değerler sayısal olarak hesaplanmıştır.

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1. Introduction

Chemical graph theory is a field of study that deals with the mathematical modeling of chemical compounds and drugs using graph theory. Designing drugs in a short time and with the least cost has become an important issue in science for diseases that have recently increased and spread rapidly. In particular, mathematicians have focused on graph invariants (topological indices) to predict the properties of chemical structures without experiments. By using graph invariants in quantitative structure-property/activity relationship studies, equations are obtained that can predict the properties of chemical structures. Molecular graphs are images of the hydrogen-free 2-D of chemical structures. The vertices of a molecular graph are represented by atoms, and the edges of the graph are represented by bonds. Topological indices are numerical descriptors of molecular graphs (Estrada and Bonchev, 2013).

The first index used to predict the properties of chemicals was the Wiener index which depends on the distance between the vertices in the graph (Wiener, 1947). The most studied indices are degree-dependent indices. Degree-dependent indices are the best predictors and the most studied indices in QSPR studies (Ediz et al., 2021; Wazzan and Urlu Özen, 2023). The first of these is the Zagreb indices defined by Gutman (Gutman, 1972). Then, various versions of the Zagreb index were introduced and studied. Some of them are the Zagreb coindex, multiplicative Zagreb index and coindex, Zagreb energy (see (Das et al., 2016; Nacaroğlu and Maden, 2017; Yalçın and Kılıç, 2021; Sevgi et al., 2022)). With this motivation, Milicevic et al. defined reformulated Zagreb indices, the edge version of Zagreb indices (Milicevic et al., 2004).

Properties and bounds of reformulated Zagreb indices were obtained (De, 2012; Maji et al., 2021). The reformulated Zagreb indices of special graphs were studied (Ji et al., 2014; Mirajkar, 2017; Liu et al., 2019). Asok and Kureethara found that the first reformulated Zagreb index for the surface tension of butane derivatives is a good estimator (Asok and Kureethara, 2018). Kaya Gök investigated bounds for reformulated Zagreb indices and coindices (Kaya Gök, 2019).

Cycle-related graphs are found in the graph representations of networks and chemicals. Sawmya calculated degree-based indices of the cycle-related chemical structures (Sawmya, 2020). Natarajan found the 2-distance vertex degree sums of cycle-related graphs (Natarajan, 2022). The values of the degree-based indices of the cycle-related graphs were calculated (see; Basavanagoud et al., 2019; Javid et al., 2020).

Various indices of phenylenes, which are nanostructures containing cycles, have been studied. The value of the Padmakar-Ivan index and the Szeged index of multiple and linear phenylenes were obtained (Yousefi-Azari et al., 2007). The Gutman index and Schultz index of random phenylene chains were studied (Wei et al., 2021). Forgotten and Co-Forgotten indices of linear [n]-phenylenes and cyclic phenylenes were studied (Havare, 2022).

In this paper, firstly, the values of reformulated Zagreb indices of wheel graph, helm graph, gear graph, friendship graph, closed helm graph, flower graph, sun, and sunflower graphs are computed. The values of the first and second Zagreb indices of these graphs are compared graphically. The rates of increase of reformulated Zagreb index values of graphs with the same edge cardinality among these graphs are compared. Finally, reformulated Zagreb indices of linear [n]-phenylenes which are cyclic chemical structures are calculated. The values of the first and second reformulated Zagreb indices for this chemical structure are compared.

2. Materials and Method

Let Γ be a graph with a vertex set $V(\Gamma)$ and edge set $E(\Gamma)$ or E. The cardinality of a vertex set and edge set is denoted as $|V(\Gamma)| = n$ and $|E(\Gamma)| = m$, respectively. The degree of a vertex, v, is the number of adjacent vertices and is denoted by d_v. The degree of an edge, $e = uv$, connected to two adjacent vertices is represented by d_e. The degree of an edge is the number of adjacent edges, i.e. $d_e = d_u + d_v - 2$. Two edges that share the same vertex are called adjacent edges. The two adjacent edges are denoted by $e \sim f$. (Gallian, 2007). See (Gallian, 2007) for the following definitions.

Definition 2.1. The cycle graph is a 2-regular graph with a vertex degree of 2 and an edge degree of 2. The number of vertices and the number of edges are equal to each other.

Definition 2.2. The wheel is a graph obtained by connecting each vertex of the cycle graph with edges from a central vertex.

Definition 2.3. The helm is a graph obtained by adding one-degree vertices to each vertex of the wheel graph's cycle graph.

Definition 2.4. The gear is formed by adding a vertex between the two vertices in the wheel graph's cycle graph.

Definition 2.5. The friendship graph is obtained by combining cycle graphs with 3-vertices from a common vertex.

Definition 2.6. A closed helm is obtained by connecting the vertices in the wheel graph's cycle with vertices in a cycle graph with an edge.

Definition 2.7. The flower is a graph obtained by combining the one-degree vertices of the helm graph and the central vertex with an edge.

Definition 2.8. The sun (crown) graph is obtained by adding pendant edges to the vertices of the cycle graph.

Definition 2.9. The sunflower graph is obtained by combining every two adjacent vertices in the cycle of the wheel with a vertex and two edges.

Definition 2.10. The first reformulated Zagreb index and the second Reformulated Zagreb index of a Γ graph, respectively, are defined as follows (Milicevic et al, 2004):

$$RM_1(\Gamma) = \sum_{e \in E} {d_e}^2 \tag{1}$$

$$RM_2(\Gamma) = \sum_{e \sim f} d_e d_f \tag{2}$$

3. Main Results and Discussion

In this section, it is obtained exact formulas for reformulated Zagreb indices of cycle-related graphs which are wheel graph, helm, gear, friendship, closed-helm, flower, sun, and sunflower graphs. Then, reformulated Zagreb indices of linear [n]-phenylenes, which have an important place in chemistry, are studied.

3.1. The Reformulated Zagreb Indices of Cycle-Related Graphs

In this section, the first and second reformulated Zagreb indices of wheel, helm, gear, friendship, closed-helm, flower, sun, and sunflower graphs are calculated, and their graphics are obtained with MATLAB program and are discussed.

Theorem 3.1.1. Reformulated Zagreb indices of the wheel graph, W, with $n+1$ vertices and $2n$ edges are:

i) $RM_1(\mathrm{W}) = n^3 + 2n^2 + 17n$

ii) $RM_2(\mathrm{W}) = \frac{n^4+n^3+15n^2+47n}{2}$.

Proof: From Definition 2.2, the edge set of the wheel graph can be partitioned as in Table 1.

Table 1. The edge degree partitions of the wheel graph

d_e for $e \in E$	Frequency
4	n
$n+1$	n

From Table 1 and the equation (1), proof (i) is completed. Table 2 depicts the edge degrees and frequency of the adjacent edges of the wheel graph.

Table 2. The adjacent-edge degree partitions of the wheel graph

(d_e, d_f) for $e, f \in E$	Frequency
$(4,4)$	n
$(4, n+1)$	$2n$
$(n+1, n+1)$	$\frac{n(n-1)}{2}$

From Table 2 and equation (2), proof (ii) is completed.

Theorem 3.1.2. Reformulated Zagreb indices of helm graph, H, with $2n+1$ vertices and $3n$ edges are:

i) $RM_1(\mathrm{H}) = n^3 + 4n^2 + 49n$

ii) $RM_2(\mathrm{H}) = \frac{n^4+3n^3+30n^2+200n}{2}$.

Proof. It can be partitioned edge degree of the edge set of the helm graph as Table 3.

Table 3. The edge degree partitions of the helm graph

d_e for $e \in E$	Frequency
3	n
$n+2$	n
6	n

From Table 3 and equation (1), proof (i) is completed. The edge degrees and frequency of the adjacent edges of the helm graph are given in Table 4.

Table 4. The adjacent-edge degree partitions of the helm graph

(d_e, d_f) for $e, f \in E$	Frequency
(3,6)	$2n$
(6,6)	n
$(3, n+2)$	n
$(6, n+2)$	$2n$
$(n+2, n+2)$	$\frac{n(n-1)}{2}$

From Table 4 and equation (2), proof (ii) is completed.

Theorem 3.1.3. Reformulated Zagreb indices of gear graph, G, with $2n+1$ vertices and $3n$ edges are:

i) $RM_1(\mathrm{G}) = n^3 + 2n^2 + 19n$

ii) $RM_2(\mathrm{G}) = \frac{n^4+n^3+11n^2+47n}{2}$

Proof. It can be partitioned edge degree of the edge set of the gear graph as in Table 5.

Table 5. The edge degree partitions of the gear graph

d_e for $e \in E$	Frequency
3	$2n$
$n+1$	n

From Table 5 and the equation (1), proof (i) is completed. Table 6 shows the edge degrees and frequency of the adjacent edges of the gear graph.

Table 6. The adjacent-edge degree partitions of the gear graph

(d_e, d_f) for $e, f \in E$	Frequency
(3,3)	$2n$
$(3, n+1)$	$2n$
$(n+1, n+1)$	$\frac{n(n-1)}{2}$

From Table 6 and the equation (2), the proof (ii) is completed.

Theorem 3.1.4. Reformulated Zagreb indices of friendship graph, fr, with $2n+1$ vertices and $3n$ edges are:

i) $RM_1(fr) = 8n^3 + 4n$

ii) $RM_2(fr) = 8n^4 - 4n^3 + 8n^2$

Proof. It can be partitioned edge degree of the edge set of friendship graph as Table 7.

Table 7. The edge degree partitions of the friendship graph

d_e for $e \in E$	Frequency
2	n
$2n$	$2n$

From Table 7 and the equation (1), the proof (i) is completed. The edge degrees and frequency of the adjacent edges of friendship graph are given in Table 8.

Table 8. The adjacent-edge degree partitions of the friendship graph

(d_e, d_f) for $e, f \in E$	Frequency
(2,2n)	$2n$
$(2n, 2n)$	$(2n-1)n$

From Table 8 and the equation (2), the proof (ii) is completed.

Theorem 3.1.5. Reformulated Zagreb indices of closed-helm graph, CH, with $2n+1$ vertices and $4n$ edges are:

i) $RM_1(CH) = n^3 + 4n^2 + 81n$

ii) $RM_2(CH) = \frac{n^4+3n^3+34n^2+368n}{2}$

Proof. It can be partitioned edge degree of the edge set of closed-helm graph as Table 9.

Table 9. The edge degree partitions of the closed-helm graph

d_e for $e \in E$	Frequency
4	n
5	n
6	n
$n+2$	n

From Table 9 and the equation (1), the proof (i) is completed. Table 10 depicts the edge degrees and frequency of the adjacent edges of closed-helm graph.

Table 10. The adjacent-edge degree partitions of the closed-helm graph

(d_e, d_f) for $e, f \in E$	Frequency
(4,4)	n
(4,5)	$2n$
(5,6)	$2n$
$(5, \mathrm{n}+2)$	n
$(6, \mathrm{n}+2)$	$2n$
(6,6)	n
$(n+2, \mathrm{n}+2)$	$\frac{n(n-1)}{2}$

From Table 10 and the equation (2), the proof (ii) is completed.

Theorem 3.1.6. Reformulated Zagreb indices of flower graph, fl with $2n+1$ vertices and $4n$ edges are:

i) $RM_1(fl) = 8n^3 + 8n^2 + 56n$

ii) $RM_2(fl) = 2n^4 + 6n^3 + 42n^2 + 114n$

Proof. It can be partition edge degree of edge set of flower graph as Table 11.

Table 11. The edge degree partitions of the flower graph

d_e for $e \in E$	Frequency
4	n
6	n
$2n$	n
$2n+2$	n

From Table 11 and the equation (1), the proof (i) is completed. The edge degrees and frequency of the adjacent edges of the flower graph are seen in Table 12.

Table 12. The adjacent-edge degree partitions of the flower graph

(d_e, d_f) for $e, f \in E$	Frequency
$(4,6)$	$2n$
$(4,2n)$	n
$(4,2n+2)$	n
$(6,2n+2)$	$2n$
$(6,6)$	n
$(2n+2,2n+2)$	$\frac{n(n-1)}{2}$
$(2n, 2n+2)$	n

From Table 12 and the equation (2), the proof (ii) is completed.

Theorem 3.1.7. Reformulated Zagreb indices of sun graph, S, with $2n$ vertices and $2n$ edges are

i) $RM_1(S) = 20n$

ii) $RM_2(S) = 32n$

Proof. It can be partition edge degree of edge set of sun graph as Table 13.

Table 13. The edge degree partitions of the sun graph

d_e for $e \in E$	Frequency
2	n
4	n

From Table 13 and the equation (1), the proof (i) is completed. The edge degrees and frequency of the adjacent edges of sun graph.are seen in Table 14.

Table 14. The adjacent-edge degree partitions of the sun graph

(d_e, d_f) for $e, f \in E$	Frequency
$(2,4)$	$2n$
$(4,4)$	n

From Table 14 and the equation (2), the proof (ii) is completed.

Theorem 3.1.8. Reformulated Zagreb indices of sunflower graph, Sf, with $2n+1$ vertices and $4n$ edges are:

iii) $RM_1(Sf) = n^3 + 6n^2 + 123n$

iv) $RM_2(Sf) = \frac{n^4+5n^3+55n^2+535n}{2}$

Proof. It can be partitioned edge degree of the edge set of sunflower graph as Table 15.

Table 15. The edge degree partitions of the sunflower graph

d_e for $e \in E$	Frequency
5	$2n$
8	n
$n+3$	n

From Table 15 and the equation (1), the proof (i) is completed. The edge degrees and frequency of the adjacent edges of sunflower graph are given in Table 16.

Table 16. The adjacent-edge degree partitions of the sunflower graph

(d_e, d_f) for $e, f \in E$	Frequency
(5,5)	$2n$
(5,8)	$2n$
$(5, n+3)$	$2n$
(8,8)	n
$(8, n+3)$	$2n$
$(n+3, n+3)$	$\frac{n(n-1)}{2}$

From Table 16 and the equation (2), the proof (ii) is completed.

The results of the theorems indicate that values of the second reformulated Zagreb indices grow faster than values of the first reformulated Zagreb indices. Figure 1 depicts the values of the first reformulated Zagreb indices of the special graphs.

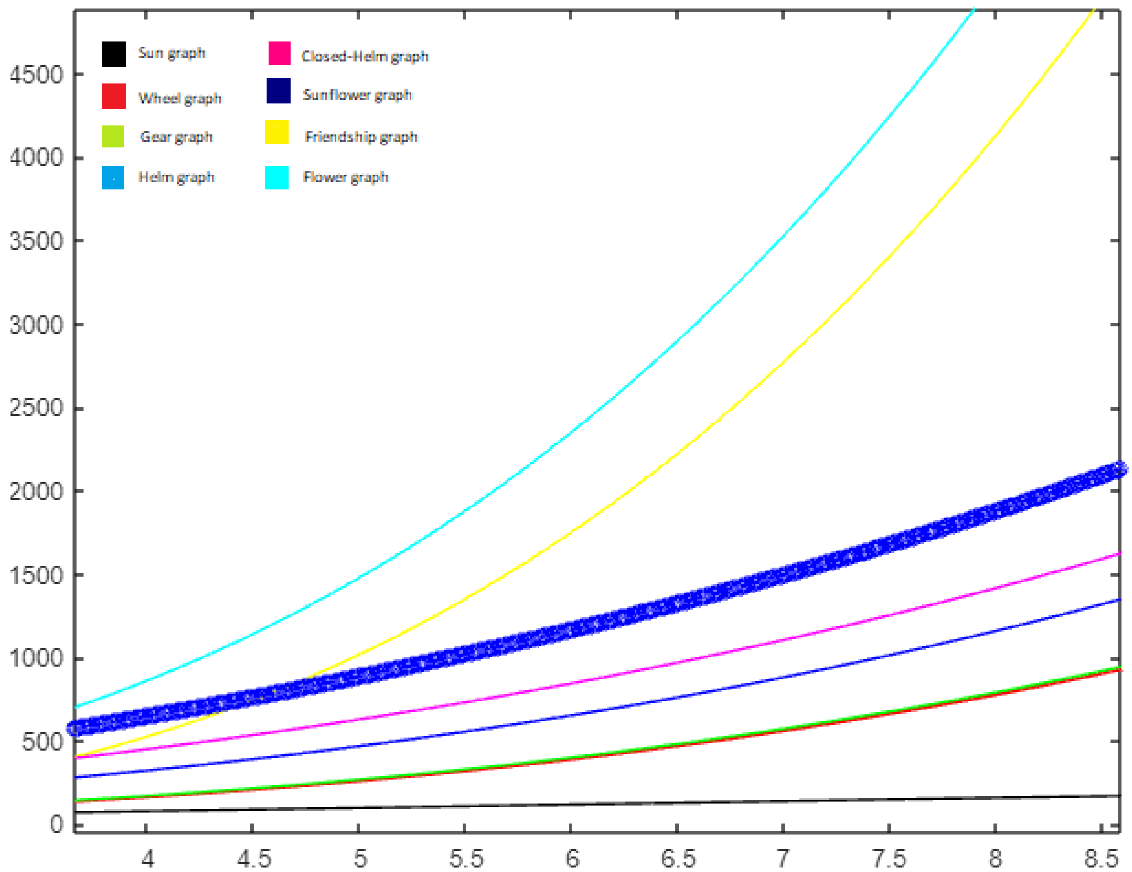


Figure 1. The reformulated first Zagreb index of cycle-related graphs

For the values of reformulated first Zagreb indices of cycle-related graphs, the value of the flower graph increases quite rapidly, then the friendship graph, sunflower, closed-helm, helm, gear, wheel, and sun graphs. The values of the gear and wheel graphs are very close to each other. The sun graph is the slowest growing and linearly increasing graph among these graphs. The edge numbers of the helm, gear, and friendship graphs are equal to each other. If these graphs are compared with each other, the graph of friendship increases very rapidly curvilinearly. The edge cardinalities of the closed-helm, flower, and sunflower graphs are equal to each other and are 4n. Figure 1 shows that the flower graph increases curvilinearly very rapidly. The number of edges of the wheel and the sun graph are equal. As the wheel graph increases curvilinearly, the sun graph increases linearly. The graphics of the second reformulated Zagreb index of the special graphs are given in Figure 2.

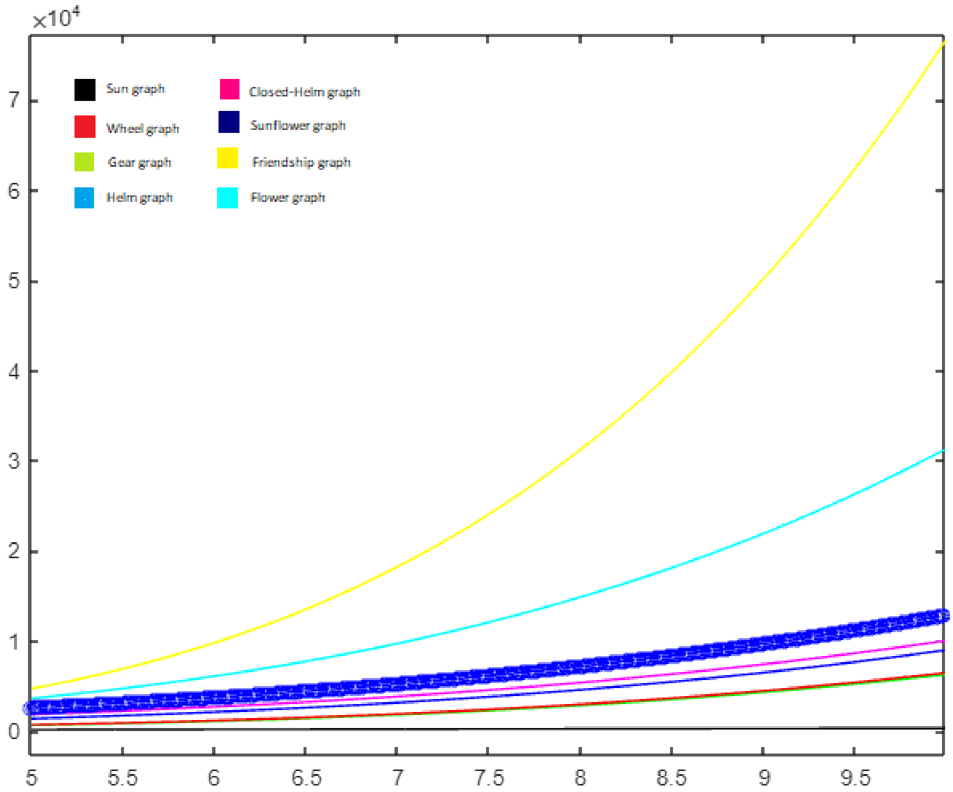
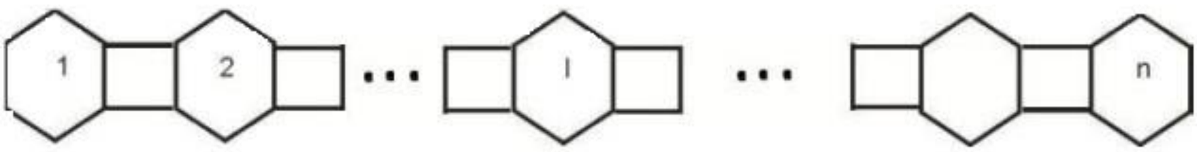


Figure 2. The second reformulated Zagreb indices of cycle-related graphs

Figure 2 shows that all graphs grow curvilinearly except the sun graph. The fastest-growing values are friendship graph. Then they are listed as flower, sunflower, closed-helm, helm, wheel, gear, and sun graph. Helm, gear, and friendship graphs with equal numbers of edges grow at different rates as n increases, and the order of their growth rates is the same as in the first reformulated Zagreb index. Similarly, the edge cardinalities of the closed-helm, flower, and sunflower graphs are the same, and the order of the growth rates of the second reformulated Zagreb indexes of these graphs is the same as that of the first reformulated Zagreb indices. The results of the gear graph and the wheel graph are very close to each other, and the growth rate of the wheel graph is larger.

3.2. Reformulated Zagreb Indices of Linear [n]-phenylenes

In this section, reformulated Zagreb indices of linear [n]-phenylenes are obtained. The molecular graphs of linear [n]-phenylenes have cycle graphs. These cycles are 6 vertices and 4 vertices. Figure 3 is a 2-D image of linear [n]-phenylenes.



Figüre 3. The linear [n]-phenylenes (Yousefi-Azari, 2007).

From Fig.3, linear [n]-phenylenes have $6n$ vertices and $6n + 2(n - 1) = 8n - 2$ edges. The partitions of edge degrees of the edge set and partitions of the edge degrees of the adjacent edges of molecular graphs of linear [n]-phenylenes are seen in Table 17 and Table 18, respectively. Let Γ be linear [n]-phenylenes graph and E be the edge set of Γ.

Table 17. The edge degree partitions of the linear [n]-phenylenes graph

d_e for $e \in E$	Frequency
2	6
3	$4n - 4$
4	$4n - 4$

Table 18. The adjacent-edge degree partitions of the linear [n]-phenylenes graph

(d_e, d_f) for $e, f \in E$	Frequency
(2,2)	4
(2,3)	4
(3,3)	$2(n - 2)$
(3,4)	$8(n - 1)$
(4,4)	$4(n - 1)$

Then, From Table 17 and Equation (1), and Table 18 and Equation (2), the following equations are obtained, respectively.

i) $RM_1(\Gamma) = 100n - 76$

ii) $RM_2(\Gamma) = 178n - 156$

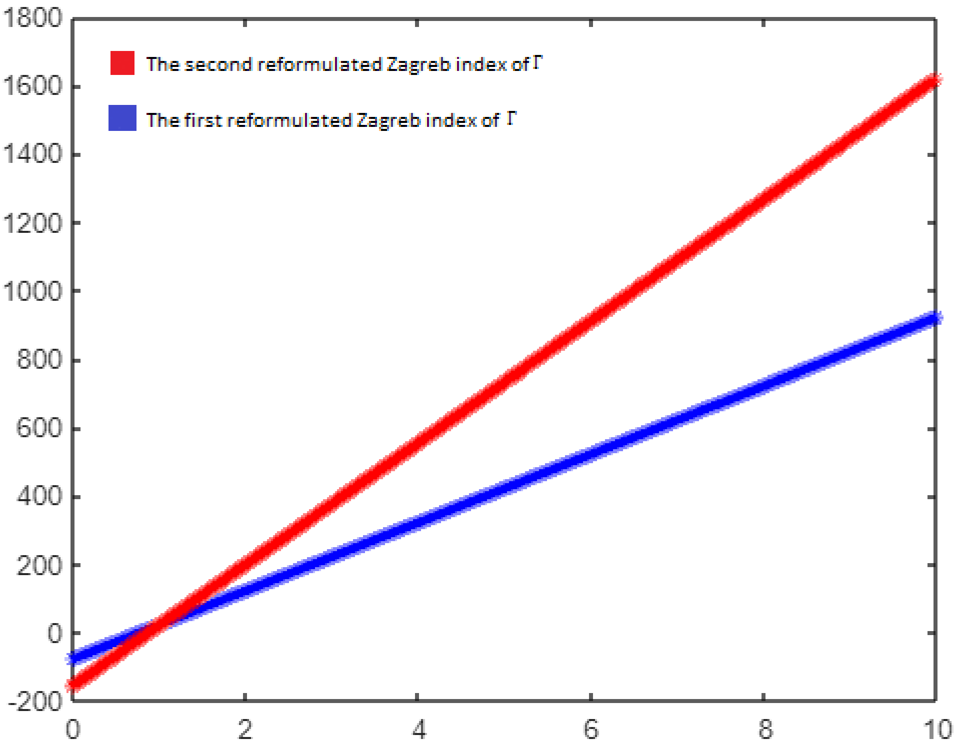


Figure 4. İndicates a graphic of reformulated Zagreb indices of linear [n]-phenylenes graphs.

As with the sun graph, the linear [n]-phenylene graph grows at linear speed as n increases. Figure 4 indicates that the values of the second reformulated Zagreb index have faster growth than the first reformulated Zagreb index.

4. Conclusion

In this paper, cycle-related graphs that are frequently encountered in computer science, communication network, and chemical graph theory are examined. These graphs are wheel, helm, gear, friendship, closed-helm, flower, sun, and sunflower. It is focused on reformulated Zagreb indices, one of the topological indices used to obtain equations to predict the physicochemical and bioactivity properties of molecules in a short time and cost-free without experimentation. Reformulated Zagreb indices of cycle-related graphs and linear [n]-phenylenes are calculated.

The results show that graphs with the same edge cardinality have different values of reformulated Zagreb indices. It is also seen that the values of the reformulated second Zagreb index are growing more rapidly than the values of the first reformulated Zagreb indices. While the fastest growing cycle-related graph is the flower graph in the first reformulated Zagreb indices, it is the friendship graph in the second reformulated Zagreb indices. While the edge cardinalities of the wheel and gear graphs are different, the value of the gear graph in the first reformulated Zagreb index is greater than the wheel graph, and the opposite in the second reformulated Zagreb indices. However, in both cases, they get very close results. The first and second reformulated Zagreb indices of the linear [n]-phenylenes with 6-vertices and 4-vertices cycles increase linearly.

The results of this study can be used to predict the properties of drugs in drug discovery. In the future studies, a quantitative structure study of cycle-related chemical structure is planned by using the results of this study.

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Conflict of interest

The author declares no conflict of interest.

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