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Araştırma Makalesi / Research Article

# New Formulas and New Bounds for the First and Second Zagreb Indices of Phenylenes

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**Abstract**

Graph theory is widely used to represent and analyze chemical structures. In addition, topological indices developed for graphs have a connection with the relationships of chemical structures such as physicochemical and bioactivity. Topological indices are widely used in QSPR-QSAR analysis and have found many applications in chemical graph theory. The oldest known degree-dependent topological indices are the first and second Zagreb indices. These indices have found wide application in chemical structures. Phenylenes containing aromatic and antiaromatic rings exhibit unique physicochemical properties and there is a wide variety of studies on phenylenes. In this article, we present some new formulas and lower bounds for the first and second Zagreb indices molecular structures of phenylenes. In addition, the BFS algorithm method, which is one of the graph algorithms, was used for the first time for the boundary study of chemical structures.

**Keywords:** First and second Zagreb indices, BFS algorithms, phenylenes.

# Fenilenlerin Birinci ve İkinci Zagreb İndeksleri için Yeni Formüller ve Yeni Sınırlar

**Öz**

Graf teorisi, kimyasal yapıları temsil etmek ve analiz etmek için yaygın olarak kullanılır. Ayrıca graflar için geliştirilen topolojik indeksler fizikokimyasal ve biyoaktivite gibi kimyasal yapıların ilişkileriyle de bağlantılıdır. Topolojik indeksler QSPR-QSAR analizinde yaygın olarak kullanılmaktadır ve kimyasal graf teorisinde birçok uygulama bulmuştur. Bilinen en eski dereceye bağlı topolojik indeksler birinci ve ikinci Zagreb indeksleridir. Bu indeksler kimyasal yapılarda geniş uygulama alanı bulmuştur. Aromatik ve antiaromatik halkalar içeren fenilenler benzersiz fizikokimyasal özellikler sergilemektedir ve fenilenler için çok çeşitli çalışmalar bulunmaktadır. Bu yazıda fenilenlerin birinci ve ikinci Zagreb indekslerinin moleküler yapıları için bazı yeni formüller ve alt sınırlar sunuyoruz. Ayrıca graf algoritmalarından BFS algoritması yöntemi ilk kez kimyasal yapıların sınır çalışmasında kullanılmıştır.

**Anahtar Kelimeler:** Birinci ve ikinci Zagreb indeksleri, BFS Algoritması, fenilenler.

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## 1. Introduction

Graph theory allows the generation of many useful qualitative predictions about the structure and reactivity of various compounds in chemical structures. Chemical structures can be represented as graphs and these chemical graph representations have wide applications; for example, they can be used as a basis for the representation and classification of many chemical systems Gutman and Trinajsti´c, 2005).

Phenylenes are actually a class of conjugated hydrocarbons consisting of six- and four-membered rings in which each four-membered ring is adjacent to a non-contiguous pair of hexagons (see Figure 1). Due to their aromatic and antiaromatic rings, phenylenes show unique physicochemical properties. Phenylenes, especially phenylene chains, are remarkable structures because of their excellent properties (Yang and Wang, 2019; Rashid et al., 2022). They are nanostructures that can be designed and fabricated very carefully for a wide variety of applications. If phenylene $h$ consists of a hexagon, it is called $h$-phenylene. The number of four-membered rings of $[h]$-phenylene is $h-1$. More information on the chemistry of phenylenes can be found in the reviews (Toda and Garratt, 1992; Vollhardt and Mohler, 1996). These discoveries in the experimental chemistry of the phenylenes opened new avenues for a great deal of theoretical investigation (Faust et al., 1992; Marković and Gutman, 1999).

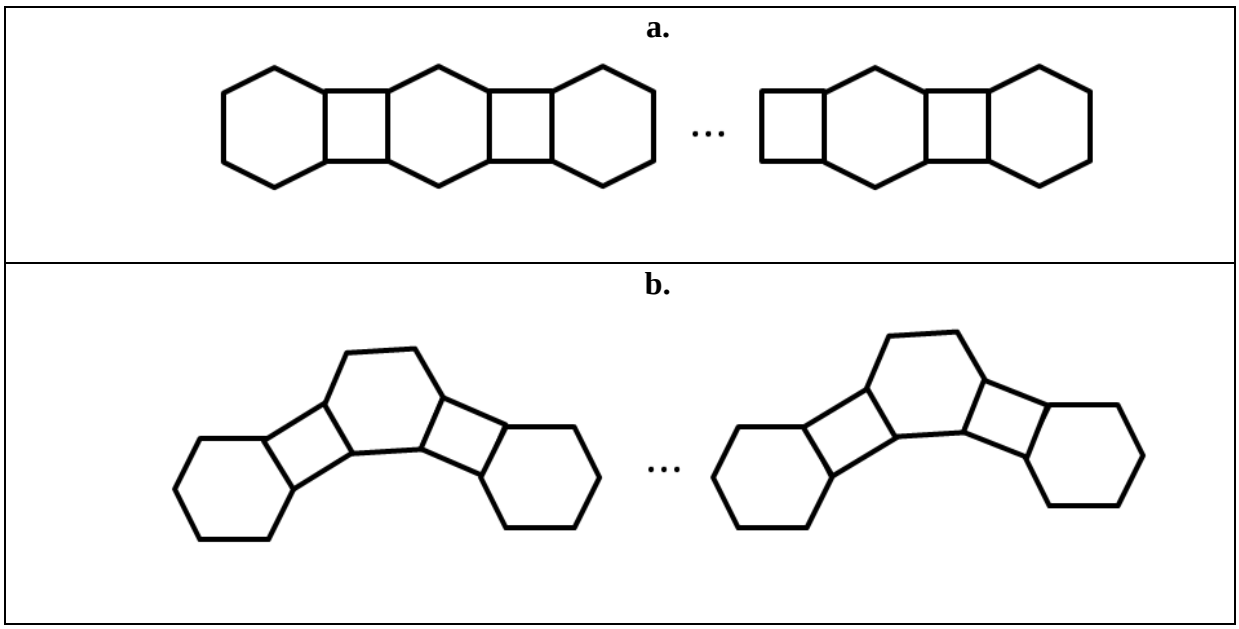


**Figure 1. a.** A lineer phenylene chain **b.** A zigzag phenylene chain (Wu, 2016)

In the graph structure of a chemical structure, the vertices represent atoms and the edges represent chemical bonds and a numerical value calculated mathematically using a molecular graph is called a topological index (Rashid et al., 2022). Topological indices based on degree and distance

are highly used in the mathematical process of combining chemical structure with physical attributes, chemical reactivity or biological activity (Jacob et al., 2023). The first known topological index was introduced in the study of boiling points of paraffin structures introduced by Wiener (Wiener, 1947). Subsequently, studies on topological indices have been proceeded by many researchers (Havare & Havare, 2022; Havare, 2024; Yousefi-Azari et al., 2024). Degree-based topological indices occupy a large place among them due to their ease of formulation and their widespread use in modeling the physicochemical properties of molecules (Das and Mondal, 2023). The first and second Zagreb indices are graph topological indices introduced by Gutman and Trinajstić. These indices are degree-dependent topological indices that were first known and widely used at chemical graph theory. The Zagreb indices and its variants have been used to study molecular complexity, chirality, quantitative structure-property/activity relationships (QSPR/QSAR) and multilinear regression models (Feng and Hu, 2011). The First and Second Zagreb indices $M_1(G)$ and $M_2(G)$ respectively are defined as follows:

$$M_1(G) = \sum_{i \in V(G)} {d_i}^2$$

$$M_2(G) = \sum_{ij \in E(G)} d_i d_j$$

where the number of edges joining one vertex $i$ to other vertices is called the degree of $i$ and is denoted by $d_i$. So far, too many inequalities have been proven regarding these indices formulas and bounds. In this study, we give various formulas for the first and second Zagreb indices of phenylene structures and then find lower and upper bounds for the first and second Zagreb indices of phenylene structures and support them with proofs. And note that, we use BFS graph algorithm method firstly, to determine upper and lower bounds of mentioned topological indices of the molecular graph structure phenylenes.

## 2. Materials and Methods

### 2.1. BFS Algorithms

Search problems frequently take the form of graph search problems, which can be solved by exploring a space of possible solutions in a systematic order (Çölkesen, 2015; Eryaşar ve Büyükköse, 2023; Everitt ve Hutter, 2015). The most commonly used search methods are BFS (breadth-first search) and DFS (depth-first search) algorithms. BFS is employed to identify connected components, assess bipartiteness, and compute shortest paths based on the number of edges (Scheffler, 2022). Similarly, DFS is utilized to locate doubly connected components in undirected graphs, strongly

connected components in directed graphs, and topological orders of directed acyclic graphs (Hopcroft and Tarjan, 1973).

Breadth First Search (BFS) is a graph search algorithm and has a special importance among graph algorithms. The BFS algorithm is widely used in countless applications and even in daily life. The BFS algorithm is widely used even in everyday life in structures such as GPS systems and to find a series of paths between two vertices whose lengths are in a certain range (Yoo et al., 2005). This algorithm works based on the neighborhood of a point. First, a starting point is selected, then each starting point adjacent to this starting point is visited (Figure 2). Based on any feature for these visited points (graph corner point naming, etc.), all running points of that point are visited from a new point. The process continues until all vertices of the graph are visited (Eryaşar and Büyükköse, 2023). The tree graph obtained as a result of this circulation is called the BFS tree.

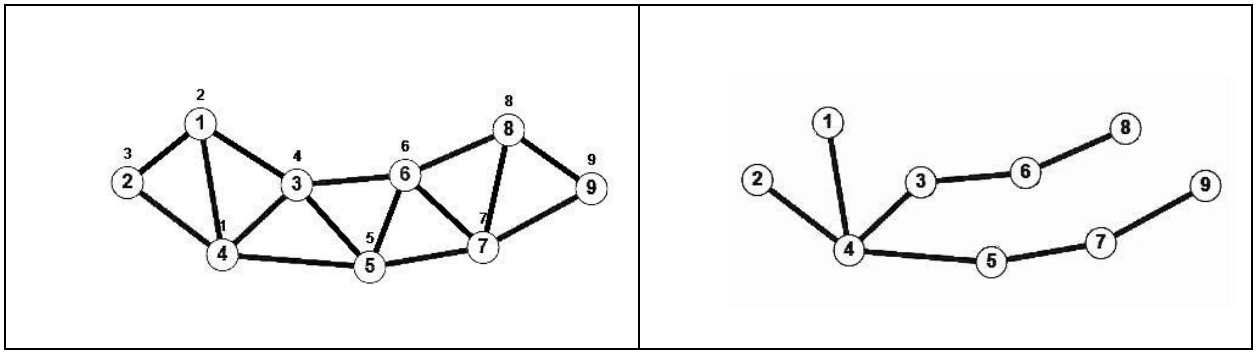

**Figure 2.** Application of BFS algorithm and formed BFS tree

In this study, lower and upper bound theorems have been developed for these structures, owing to the tree structure obtained as a result of applying the BFS algorithm to the graph representation of phenylene structures. When applying the BFS algorithm, we start with one of the vertices with the largest initial degree (represented by Δ) (Figure 3).

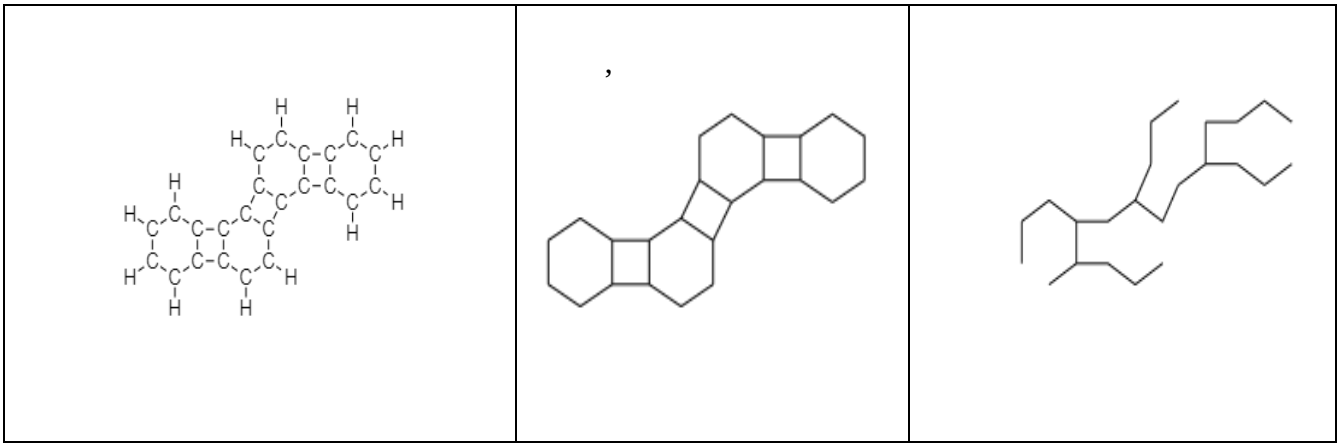

**Figure 3.** Example of phenylene and BFS tree presented with structural formulas and corresponding molecular graphs (Marković et al., 2001)

## 3. Findings and Discussion

### 3.1. First and Second Zagreb Indices of Phenylenes

**Lemma 1.** If a phenylene structure consists of $m$ squares and $n$ hexagons, then the number of vertices for the graph structure of phenylene is $6n$ and the number of edges is $6n + 2m$.

**Theorem 1.** Let a phenylene structure with $v$-point consists of $n$ hexagons and $m$ squares. Then,

$$M_1(G) = 4(5m + v)$$

and

$$M_2(G) = 3(3v - r - 14) - 5s\,.$$

*Proof.*

For a phenylene structure, each vertex of the squares have the degrees 3, and vertices outside the square corners of the hexagon have the degrees 2, thus

$$M_1(G) = 4m(3^2) + (v - 4m)(2^2)$$
$$= 4(5m + v).$$

Firstly note that $r$ and $s$ will represent the number of edges $E_{2,3}$ and $E_{2,2}$, respectively where $E_{i,j} = \{d_u = i \text{ and } d_v = j\}$.

Let us do the proof for an $w$ −edged phenylene considering the edges. For only a square in a phenylene structure since each of the corner points has the degree 3, then there are four $E_{3,3}$. For a phenylene structure containing $m$-squared, the number of the edges $E_{3,3}$ is $4m$. Also, three-$E_{2,2}$ and two-$E_{2,3}$ will come from the end hexagons of each phenylene structure. Thus $4m.(3.3) + [3(2.2) + 2(2.3)] = 36m + 48$ is constant. Finally, the remaining $(w - 4m - 10 - r - s)$ edges are $E_{3,3}$, therefore

$$M_2(G) = 36m + 48 + 6r + 4s + (w - 4m - r - s - 10)9$$
$$= 9v - 3r - 5s - 42$$
$$= 3(3v - r - 14) - 5s.$$

### 3.2. New Lower and Upper Bounds for the First and Second Zagreb Indices of Phenylenes Structure with the help of BFS Algorithm

**Theorem 2.** For a phenylenes graph structure with $v$-points, there is an inequality as follows:

$$(\Delta^2 - 4)k - 6n + 4v \leq M_1(G)$$

where $n$ is the total number of hexagons in phenylene, $\Delta$ is the maximum degree for the BFS tree of the phenylene graph structure, and $k$ is the maximum number of ordered points for the same tree.

*Proof.*

If the BFS algorithm is applied to a phenylene graph structure, a BFS tree is obtained. A phenylene is a structure made of hexagons and squares. Since the degree 3 is the maximum of the existed degrees in this structure, let take any point with the degree 3 as a starting point. Let there be $k$ points of degree $\Delta$ in the BFS tree of phenylene. All remaining points will have the degrees 1 or 2. If there are $n$ hexagons in the phenylene structure, assume that phenylene has maximum $2n$-points in the BFS tree having degree 1. Therefore, the remaining $v-k-2n$ points are of degrees 2, hence

$$k\Delta^2 + 2n(1^2) + (v-k-2n)2^2 \leq k\Delta^2 + 2n + 4v - 4k - 8n$$
$$\leq (\Delta^2 - 4)k - 6n + 4v \leq M_1(G).$$

**Theorem 3.** For a phenylenes graph structure with $v$-points, there is an inequality

$$2(\Delta - 2)k + 4(v-n) \leq M_2(G)$$

where $n$ is the total number of hexagons in phenylene, $\Delta$ is the maximum degree for the BFS tree of the phenylene graph structure, and $k$ is the maximum number of ordered points for the same tree.

*Proof.*

If the BFS algorithm is applied to a phenylene graph structure, a BFS tree is obtained. A phenylene is a structure made of hexagons and squares. Since the degree 3 is the maximum of the existed degrees in this structure, let take any point with the degree 3 as a starting point. If there are $n$ hexagons in the phenylene structure, assume that phenylene has maximum $2n$-points in the BFS tree having degree 1. Let the degree of each point connected to these vertices be maximum 2. Let the phenylene BFS tree has $k$ points with degree maximum $\Delta$. If we take the degrees of the vertices adjacent to these maximum degree points and the degrees of all the remaining points are of degrees 2, we get

$$(1.2)2n + (2.\Delta)k + (2.2)(v-2n-k) = 4n + 2\Delta k + 4v - 8n - 4k$$
$$= 2(\Delta - 2)k + 4(v-n) \leq M_2(G)\,.$$

**Theorem 4.** For a phenylenes graph structure with $v$-points, there is an inequality

$$2((\Delta^2 - 4)4m - 3z + 4v) \geq M_1(G)$$

where $v$ is the total number of hexagons in phenylene, $\Delta$ is the maximum degree for the BFS tree of the phenylene graph structure, and $m$ is the total number of squares.

*Proof.*

For the tree structure obtained as a result of applying the BFS algorithm to a phenylene containing $m$-squares, let $4m$ be the number of vertices ordered $\Delta$. In addition $z$ is the number of points with degree 1 and the number of points with degree 2 is $(n-4m-z)$,

$$2[4m(\Delta^2)+z1^2+(v-4m-z)2^2] = 2[4m\Delta^2+z+4v-16m-4z]$$
$$= 2[(\Delta^2-4)4m-3z+4v] \geq M_1(G).$$

**Theorem 5.** For a phenylenes graph structure with $v$-points, there is an inequality

$$4[2(m(\Delta-4)+v)-z] \geq M_2(G)$$

where $v$ is the total number of hexagons in phenylene, $\Delta$ is the maximum degree for the BFS tree of the phenylene graph structure, and $m$ is the total number of squares.

*Proof.*

If a phenylene with $v$-points contains $m$-squares, suppose that $4m$ be the number of vertices ordered $\Delta$. Let us assume that the degree of each remaining point (depending on $\Delta$, including points with degree 1) in the BFS tree structure, including the number of graduated points $z$, are 2. In that case,

$$2[4m(\Delta.2)+(1.2)z+(v-4m-z)(2.2)] = 2[8m\Delta+2z+4v-16m-4z]$$
$$= 4[2m\Delta+z+2v-8m-2z]$$
$$= 4[2m(\Delta-4)+2v-z]$$
$$= 4[2(m(\Delta-4)+v)-z] \geq M_2(G).$$

**Authors' Contributions**

All authors contributed equally to the study.

**Statement of Conflicts of Interest**

There is no conflict of interest between the authors.

**Statement of Research and Publication Ethics**

This study complies with Research and Publication Ethics.

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