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Maximal Diminished Sombor Index of Tricyclic Graphs

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Abstract

The diminished Sombor index of a graph G with edge set E is defined as

$$DSO(G) = \sum_{uv \in E} \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v},$$

in which d_u and d_v are the degrees of the adjacent vertices u and v, respectively.

In this note, we determine the unique tricyclic graph of a given order maximizing DSO, and characterize some structural properties of this graph.

1 Introduction

Chemical graph theory is a branch of mathematics that models molecular structures as graphs, where vertices represent atoms and edges correspond to chemical bonds. Within this framework, topological indices have emerged as essential numerical descriptors that capture structural features of molecules and are widely used in quantitative structure–activity

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(QSAR) and structure–property (QSPR) relationship studies. Among these, degree-based indices are particularly valued for their computational simplicity and strong correlation with chemical phenomena.

Consider a simple graph G with vertex set $V(G)$ and edge set $E(G)$. The order of G is $|V(G)| = n$ and its size of G is $|E(G)| = m$. An edge between two vertices u and v is denoted by uv, while the degree of a vertex $u \in V(G)$, written as d_u, corresponds to the number of vertices in G that are adjacent to u [5].

In 2021, Gutman [4] introduced the Sombor index as a novel degree-based invariant, defined for a graph G as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}.$$

For further details on the properties and applications of Sombor indices, refer to [3, 6–8, 11].

Rajathagiri [10] proposed the diminished Sombor index (DSO), a normalized variant given by

$$DSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v}.$$

This index was further investigated by Movahedi et al. [9] who demonstrated its strong predictive ability for various physicochemical properties and explored its mathematical properties in depth.

A central problem in the study of topological indices is the identification of extremal graphs, those that maximize or minimize a given index within a specified graph family. Previous research determined extremal graphs for the DSO index among trees, unicyclic, and bicyclic graphs [9]. These developments highlight the complexity and ongoing interest in extremal problems for the DSO index within tricyclic graph families. Das et al. [2] determined the graph with the minimum diminished Sombor index of tricyclic graphs.

The present paper addresses the open problem of maximizing the DSO index among tricyclic graphs. We identify the unique tricyclic graph of

order n that attains the absolute maximum DSO. Furthermore, we provide a complete characterization of tricyclic molecular graphs (those with maximum vertex degree at most 4) that maximize the DSO index.

2 Main results

In this section, we present the main results of this paper.

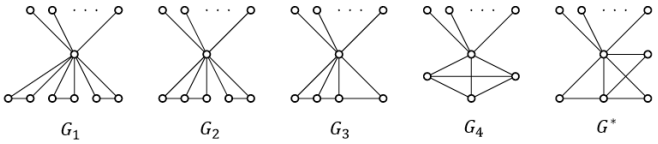

Figure 1. All tricyclic graphs of order n and maximum degree $n-1$.

Theorem 1. *The graph G^* shown in Figure 1 is the unique tricyclic graph of order $n \geq 5$ that attains the maximum diminished Sombor index.*

Proof. Similar to the discussion in [9], we consider the function $f(x,y) = \frac{\sqrt{x^2+y^2}}{x+y}$ such that $x, y \in [1, n-1]$. The partial derivatives of the function for $x > y$ in the interval $[1, n-1]$ are positive with respect to x and negative with respect to y. Therefore, the maximum value of the function is attained as follows

$$f(x,y)_{max} = f(n-1,1) = \frac{\sqrt{(n-1)^2+1}}{n}.$$

Consequently, it suffices to examine all tricyclic graphs of order n whose maximum degree is $n-1$. These graphs, specifically G_i for $i = 1,2,3,4$ and G^*, are depicted in Figure 1. The DSO index for G_1, G_2, G_3, G_4, and G^* are listed below, respectively

$$DSO(G_1) = \frac{3\sqrt{2}}{2} + 6\left(\frac{\sqrt{(n-1)^2+4}}{n+1}\right) + (n-7)\left(\frac{\sqrt{(n-1)^2+1}}{n}\right),$$

$$DSO(G_2) = \frac{2\sqrt{13}}{5} + \frac{\sqrt{2}}{2} + (n-6)\left(\frac{\sqrt{(n-1)^2+1}}{n}\right)$$

$$+4\left(\frac{\sqrt{(n-1)^2+4}}{n+1}\right)+\frac{\sqrt{(n-1)^2+9}}{n+2},$$

$$DSO(G_3)=\frac{2\sqrt{13}}{5}+\frac{\sqrt{2}}{2}+2\left(\frac{\sqrt{(n-1)^2+4}}{n+1}\right)+2\left(\frac{\sqrt{(n-1)^2+9}}{n+2}\right)$$
$$+(n-5)\left(\frac{\sqrt{(n-1)^2+1}}{n}\right),$$

$$DSO(G_4)=\frac{3\sqrt{2}}{2}+(n-4)\left(\frac{\sqrt{(n-1)^2+1}}{n}\right)+3\left(\frac{\sqrt{(n-1)^2+9}}{n+2}\right),$$

$$DSO(G^*)=\sqrt{5}+(n-5)\left(\frac{\sqrt{(n-1)^2+1}}{n}\right)+3\left(\frac{\sqrt{(n-1)^2+4}}{n+1}\right)$$
$$+\frac{\sqrt{(n-1)^2+16}}{n+3}.$$

A comparison between each of the initial four expressions and the final one shows that $DSO(G_i) < DSO(G^*)$ holds for $n \geq 5$ and for any $i \in \{1,2,3,4\}$. ■

To conclude, we present a result regarding the maximum diminished Sombor index among tricyclic molecular graphs, which is derived from Theorem 2 of [1].

Theorem 2. *Let G be a tricyclic molecular graph of order $n \geq 11$. Then the graphs attaining the maximum diminished Sombor index can be characterized as follows*

(i) If $n \equiv 0 \pmod 3$, the maximum is attained only by graphs that contain exactly one vertex of degree 2, which is adjacent to two vertices of degree 4, and contain no vertex of degree 3.

(ii) If $n \equiv 1 \pmod 3$, the extremal graphs are those that have exactly one vertex of degree 3, connected to three vertices of degree 4, and no vertex of degree 2.

(iii) If $n \equiv 2 \pmod 3$, the maximum is achieved exclusively by graphs with no vertices of degree 2 or 3.

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