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Bounds and extremal graphs of second reformulated Zagreb index for graphs with cyclomatic number at most three

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Abstract

Miličević *et al.*, in 2004, introduced topological indices known as Reformulated Zagreb indices, where they modified Zagreb indices using the edge-degree instead of vertex degree. In this paper, we present a simple approach to find the upper and lower bounds of the second reformulated Zagreb index, $EM_2(G)$, by using six graph operations/transformations. We prove that these operations significantly alter the value of reformulated Zagreb index. We apply these transformations and identify those graphs with cyclomatic number at most 3, namely trees, unicyclic, bicyclic and tricyclic graphs, which attain the upper and lower bounds of second reformulated Zagreb index for graphs.

Keywords: Bicyclic graphs; trees; tricyclic graphs; unicyclic graphs; reformulated Zagreb index.
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1. Introduction

Topological indices play a crucial role in characterizing the properties of molecules in terms of physical, chemical and biological. Several types of topological indices exist in mathematical chemistry, such as the Wiener index (Wiener, 1947); Hyper Wiener index (Klein *et al.*, 1995); Hosoya index (Hosoya, 1971); Randić index (Randić, 1975); Augmented Zagreb index (Furtula *et al.*, 2010); Harmonic index (Fajtlowicz, 1987); to name a few. For more details on topological indices, we refer to some articles here (Basak, 2016; Devillers & Balaban, 2000; Gutman, 2013; Gutman *et al.*, 2014, 2020; Karelson, 2000; Narayankar *et al.*, 2020; Rada & Bermudo, 2019; Romero-Valencia *et al.*, 2019; Shang, 2016; Varmuza *et al.*, 2012).

Throughout this paper, we consider only non trivial simple connected graphs. Let a simple connected graph of n vertices be denoted by $G = (V(G), E(G))$, where $V(G)$ and $E(G)$ denote the set of vertices and set of edges of the graph respectively. Let $d_G(u)$ denote the *degree of the vertex* u, $d_G(e)$ denotes the *degree of the edge* e. $N_G(u) = \{v \in V(G) : uv \in E(G)\}$ denotes the set of all *neighbours* of vertex u in G, that is, $d_G(u) = |N_G(u)|$. The cyclomatic number of a graph is defined as $cy(G) = |E(G)| - |V(G)| + 1$. Trees have no cycles and hence has cyclomatic number to be 0. When $m = n$, G has cyclomatic number 1 and called as a *unicyclic graph*. When $m = n + 1$, G has cyclomatic number 2 and referred to as *bicyclic graph*. When $m = n + 2$, G has cyclomatic number 3 and referred to as *triyclic graph*. Let S_n, P_n, and C_n denoted the star graph, path graph, and cycle graph of n vertices. Other notations and definitions are taken from the book (Bondy *et al.*, 1976).

The Zagreb indices are one of the most important and well studied topological indices in the literature. It first appeared in 1972, during the study of $\pi-$energy of conjugate molecules. For a simple graph G, Zagreb indices (Gutman & Das , 2004; Gutman & Trinajstić , 1972) are defined as

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