

Comparing Zagreb Indices

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Let G be a simple graph. Denote by $V(G)$ set of its vertices, by $E(G)$ set of its edges, by $n(G)$ number of its vertices and by $m(G)$ number of its edges. The first and the second Zagreb indices are defined by: $M_1(G) = \sum_{v \in V(G)} d(v)^2$ and $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$, where $d(v) = d_G(v)$ is the degree of vertex v in the graph G .

On the IAMC meeting 2006, the following conjecture has been proposed by Pierre Hansen

Conjecture. It holds

$$M_1(G)/n(G) \leq M_2(G)/m(G) \quad (1)$$

for all simple connected graphs G . Moreover, this bound is tight.

Here it will be shown that this conjecture is generally not true, but it is true for graphs with maximal degree at most four (which has chemical significance), for acyclic graphs and for unicyclic graphs.

The inequality ${}^\lambda M_1/n \leq {}^\lambda M_2/m$ as the generalization of inequality (1) is analyzed for general graphs, graphs with maximal degree at most four and for trees.

These results are furthered by the analysis of edge-connectivities. Let $m_{ij}(G)$ be the number of edges of graph G , connecting vertices of degrees i and j . Necessary and sufficient conditions are established on a symmetric matrix of type $\Delta \times \Delta$ such that there is a tree T for which $M_{ij} = m_{ij}(T)$. These results are used in the creation of the software ChemoGraphX.