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Extremal Chemical Trees of the First Reverse Zagreb Alpha Index

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Abstract: Topological indices have important effect to develop chemical sciences by using graph invariants. The Zagreb indices are the most used topological indices in mathematical chemistry literature. Novel forms of Zagreb indices have been extensively defined in recent times. One of the latest version of the Zagreb indices is the reverse Zagreb alpha index. Extremal chemical trees with respect to Zagreb indices have been studied many times in the last two years. In this paper maximum chemical trees were characterized with respect to the first reverse Zagreb alpha index.

Keywords: Reverse Zagreb Indices, Zagreb Indices, Topological Index, The First Zagreb Alpha Index, The First Zagreb Beta Index, The Second Reverse Zagreb Index

1. Introduction

Graph theory which is one of the most important branches of applied mathematics has many applications related to chemical and biological sciences. These chemical and biological applications of the graph theory contribute the birth of "chemoinformatics". Chemoinformatics is the intersection of the sciences of mathematics, chemistry and informatics. In chemistry, sometimes to conduct experimental studies of materials cannot be possible because of expensiveness and complexity of large-scale materials such as chemical networks. In these situations, theoretical studies are indispensable for modelling and predicting physicochemical and biological properties of such materials, molecules and networks. In chemoinformatics literature these studies are named as "Quantitative structure-property and structure-activity relationships studies (QSPR and QSAR)". In QSAR\QSPR studies, scientists need to understand the underlying topology of chemical networks via some numerical parameters derived from the molecular graphs of these networks. These numerical parameters which defined as topological descriptors are used for modelling and prediction of physicochemical and biological features of chemical networks usually by means of correlation efficients. Among the all topological descriptors, the topological indices are most used parameters in QSAR\QSPR studies. There are many molecular topological studies in literature which showed the importance of molecular topological descriptors in QSAR\QSPR studies. Chemical graph theory has an important effect on the development of the chemical sciences by using topological indices. A topological index, which is a graph invariant it does not depend on the labeling or pictorial representation of the graph, is a numerical parameter mathematically derived from the graph structure. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity. These indices are used in quantitive structure property relations (QSPR) research.

Let G be a simple connected graph with n vertices and m edges. d_v is the number of edges incident to the vertex v. We write Δ and δ for the largest and the smallest of all degrees of vertices of G, respectively. Trees are connected graphs that do not contain any cycle. A tree is called chemical if no vertex of it has a degree greater than four.

The first distance based topological index was proposed by Wiener (1947) for modeling physical properties of alcanes, and after him, hundred topological indices were defined by chemists and mathematicians and so many properties of chemical structures were studied [1]. More than forty years ago Gutman & Trinajstić (1971) defined Zagreb indices which are degree based topological indices [2]. These topological indices were proposed to be measures of

branching of the carbon-atom skeleton in [3]. The first and second Zagreb indices of a simple connected graph G defined as follows;

$$M_1(G)=\sum_{u\in V(G)} d_u^2$$

And

$$M_2(G)=\sum_{uv\in E(G)} d_u d_v$$

where u, $V(G)$, uv and $E(G)$ denotes a vertex of G, the vertex set of G, an edge of G and the edge set of G, respectively. For details of the chemical applications and the mathematical theory of the Zagreb indices, see the surveys [4-8] For the another version of the first Zagreb index;

$$M_1(G)=\sum_{uv\in E(G)} (d_u+d_v)$$

see in [6, 7, 11, 13-26] and references therein for detailed discussions of Zagreb and novel Zagreb indices.

Extremal chemical trees with respect to Zagreb indices were determined in [8, 9]. Recently in [10], the extremal values of the reformulated first Zagreb index has been investigated.

Reverse Zagreb indices have been defined in [12] as follows.

The reverse vertex degree of a vertex v of a simple connected graph G defined as;

$$c_v=\Delta-d_v+1$$

where Δ denotes the largest of all degrees of vertices of G and d_v denotes the number of edges incident to v. The total reverse vertex degree defined as;

$$TR(G)=\sum_{u\in V(G)} c_u .$$

The first reverse Zagreb alpha index of a simple connected graph G defined as;

$$CM_1^{\alpha}(G)=\sum_{u\in V(G)} c_u^2 .$$

The first reverse Zagreb beta index of a simple connected graph G defined as;

$$CM_1^{\beta}(G)=\sum_{uv\in E(G)} (c_u+c_v).$$

And the second reverse Zagreb index of a simple connected graph G defined as; $CM_2(G)=\sum_{uv\in E(G)} c_u c_v$

Extremal trees and graphs with respect to total reverse vertex degree and first reverse Zagreb alpha index have been characterized in [12]. The aim of this paper is to characterize maximum chemical trees with respect to the first reverse Zagreb alpha index.

2. Maximum Chemical Trees of the First Reverse Zagreb Alpha Index

Lemma 1. Let G be a chemical tree with n vertices and for each $i\in\{n_1,n_2,n_3,n_4\}$, let n_i denote the number of vertices of degree i for $n_4>0$. Then;

$$CM_1^{\alpha}(G)=16n_1+9n_2+4n_3+n_4. \quad (1)$$

Proof. Clearly,

$$n_1+n_2+n_3+n_4=n. \quad (2)$$

From the handshaking lemma,

$$n_1+2n_2+3n_3+4n_4=2(n-1) \quad (3)$$

From the definition of the reverse vertex degree, n_1, n_2, n_3 and n_4 denotes the number of the vertices of reverse degrees 4, 3, 2 and 1, respectively for $n_4>0$. And from the definition of the first reverse Zagreb alpha index, the desired result acquired directly.

Notice that, for any chemical tree,

$$n_2+2n_3+3n_4=n-2 \quad (4)$$

can be written by using Equations 2 and 3. And, if the Equation 3 is subtracted from the five-fold of the Equations 2, then it is got that;

$$4n_1+3n_2+2n_3+n_4=3n+2 \quad (5)$$

Theorem 2. Let G be chemical tree with $n\geq 5$ vertices. Then;

$$CM_1^{\alpha}(G)=\begin{cases}11n+8, & \text{if } n\equiv 0,1 \pmod 3,\\ 11n+10, & \text{if } n\equiv 2 \pmod 3.\end{cases}$$

Proof. There are three cases.

Case 1: Let $n=3r$, $r\geq 2$. In this case the Equation 4 transforms to $n_2+2n_3+3n_4=3r-2$. And from this last equality, it was got that $n_4\leq r-1$. If for $n_4=r-1$, then $n_2=1$ and $n_3=0$. From the Equation 2, $n_1=2r$. By using the Equation 1, $CM_1^{\alpha}(G)=11n+8$. If for $n_4\leq r-2$, then from the Equation 4, it was got that the inequality,

$$4\leq n_2+2n_3\leq 3r-5 \quad (6)$$

If the Equation 5 was multiplied by four, then it was got that $16n_1+12n_2+8n_3+4n_4=36r+8$. It can be rewritten this last equality by using the Equation 1 as;

$$CM_1^{\alpha}(G)+3n_2+4n_3+3n_4=36r+8.$$

From this last equality, if it is shown that $3n_2+4n_3+3n_4>3r$ then also it is shown that $CM_1^{\alpha}(G)<33r+8=11n+8$. For this, let accept that $3n_2+4n_3+3n_4\le 3r$ especially $3n_2+4n_3+3n_4 = 3r$. It can be rewritten this last equality by using the Equation 3 as; $n_1+2n_2+3n_3+4n_4-n_1+n_2+n_3-n_4=3r$. And from this, we get that $n_1-n_2-n_3+n_4=3r-2$. If this last equality was subtracted from the Equation 2, it was got that $n_2+n_3=1$ which is a contradiction to the Inequality 6. Therefore, for $n=3r$ ($r\ge 2$), if G is n-vertex chemical tree, then $CM_1^{\alpha}(G)\le 11n+8$ and equality is attained if and only if there are $r-1$ vertices of degree 4, one vertex of degree 2 and remaining vertices are pendant.

Case 2. Let $n=3r+1$, $r\ge 2$. In this case the Equation 5 transforms to $n_2+2n_3+3n_4=3r-1$. And from this last equality, it was got that $n_4\le r-1$. For $n_4=r-1$, and there are the next two possibilities: $n_2=0$, $n_3=1$ or $n_2=2$, $n_3=0$. In the first case; $CM_1^{\alpha}(G)=11n+8$ and and in the second one $CM_1^{\alpha}(G)=11n+6$. If for $n_4\le r-2$, then from the Equation 4, the following inequality was acquired,

$$5\le n_2+2n_3\le 3r-4 . \quad (7)$$

If the Equation 5 was multiplied by four, then it was got that $16n_1+12n_2+8n_3+4n_4=36r+20$. It can be rewritten this last equality by using the Equation 1 as;

$CM_1^{\alpha}(G)+3n_2+4n_3+3n_4=36r+20$. From this last equality, if it can be shown that $3n_2+4n_3+3n_4>3r+1$ then also it was showed that $CM_1^{\alpha}(G)<33r+19=11n+8$. For this, let accept that $3n_2+4n_3+3n_4\le 3r+1$ especially $3n_2+4n_3+3n_4=3r+1$. It can be rewritten this last equality by using the Equation 3 as; $n_1+2n_2+3n_3+4n_4-n_1+n_2+n_3-n_4=3r+1$. And from this, it was got that $n_1-n_2-n_3+n_4=3r-1$.

If we subtract this last equality from the Equation 2, then it was acquired that $n_2+n_3=1$ which is a contradiction to the Inequality 7. Therefore, for $n=3r+1$ ($r\ge 2$), if G is n-vertex chemical tree, then $CM_1^{\alpha}(G)\le 11n+8$ and equality is attained if and only if there are $r-1$ vertices of degree 4, one vertex of degree 3 and remaining vertices are pendant.

Case 3. Let $n=3r+2$, $r\ge 1$. In this case the Equation 5 transforms to $n_2+2n_3+3n_4=3r$. And from this last equality, it was got that $n_4\le r$. Similarly with the above cases, for $n=r$, we have that $n_2=n_3=0$ and the first reverse Zagreb alpha index on this class of trees takes value $CM_1^{\alpha}(G)=11n+10$. Otherwise $n_4\le r-1$ and from the Equation 4, it was got that the following inequality,

$$3\le n_2+2n_3\le 3r-3. \quad (8)$$

If we multiply the Equation 5 by four, then it was got that $16n_1+12n_2+8n_3+4n_4=36r+32$. It can can rewrite this last equality by using the Equation 1 as;

$CM_1^{\alpha}(G)+3n_2+4n_3+3n_4=36r+32$. From this last equality, if we show that $3n_2+4n_3+3n_4>3r$ then also we show that $CM_1^{\alpha}(G)<33r+32=11n+10$. For this, let we accept that $3n_2+4n_3+3n_4\le 3r$ especially $3n_2+4n_3+3n_4=3r$. It can be rewritten this last equality by using the Equation 3 as; $n_1+2n_2+3n_3+4n_4-n_1+n_2+n_3-n_4=3r$. And from this, we get that $n_1-n_2-n_3+n_4=3r+2$. If we subtract this last equality from the Equation 2, then it was acquired that $n_2+n_3=0$ which is a contradiction to the Inequality 8. Therefore, for $n=3r+2$ ($r\ge 2$), if G is n-vertex chemical tree, then $CM_1^{\alpha}(G)\le 11n+8$ and equality is attained if and only if there are r vertices of degree 4 and the remaining vertices are pendant.

3. Conclusion

Reverse Zagreb indices have been defined recently. In this study, extremal chemical trees with respect to the first reverse Zagreb alpha index were determined. It can be interesting to find extremal unicyclic, bicyclic, tricyclic graphs of the reverse Zagreb indices. It can also be interesting to compute the exact values of the reverse Zagreb indices of some chemical structures such as nanotubes and nanotorus.

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