Mathematica Aeterna, Vol. 3, 2013, no. 2, 133 - 138

Reformulated Zagreb Indices of Dendrimers

Nilanjan De

Department of Basic Sciences and Humanities (Mathematics),
Calcutta Institute of Engineering and Management, Kolkata, India,
E-mail: de.nilanjan@rediffmail.com

Abstract

The reformulated Zagreb indices of a graph is obtained from the classical Zagreb by replacing vertex degree by edge degree and are defined as sum of squares of the degree of the edges and sum of product of the degrees of the adjacent edges. In this paper we give some explicit results for calculating the first and second reformulated Zagreb indices of dendrimers.

Mathematics Subject Classification: 05Cxx

Keywords: Edge Degree, Reformulated Zagreb Indices, Dendrimers.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let n be the number of vertices and m be the number of edges of G. The classical Zagreb indices, introduced by Gutman and Trinajstić [1], are defined respectively as the sum of squares of the degrees of the vertices and sum of product of the degrees of the adjacent vertices of a graph. The first and second reformulated Zagreb indices, introduced in 2004 [2] are the edge version of the classical Zagreb indices so that these pair of indices are respectively defined as

$$EM_1(G) = \sum_{e \in E(G)} d(e)^2 \quad \text{and} \quad EM_2(G) = \sum_{e \sim f} d(e)d(f)$$

where *d(e)* is the degree of the edge *e* in *G* and is defined as $d(e) = d(u) + d(v) - 2$, where *d(u)* and *d(v)* are degree of the vertices *u* and *v* and $e = (u, v)$. Also e~f means that the edges *e* and *f* share a common end vertex i.e. *e* and *f* are adjacent. In this regard reader should note that the first and second reformulated Zagreb indices are equal to first and second Zagreb indices for line graph of a graph [4].Recently some properties, upper and lower bounds of $EM_1(G)$ and $EM_2(G)$ are presented in [4] and [5]. Also in [3] the extremal values of the first reformulated Zagreb index are presented. Recently in [6] the present author gives some new lower and upper bounds of these two indices.

Dendrimers $T_{d,k}$ are hyper-brunched nanostructure considered as a central tree. Let the central vertex of dendrimers is denoted by v_0 and every non pendent vertices is of degree *d*. Also the distance of each pendent vertices of the dendrimers $T_{d,k}$ from the central vertex v_0 is *k* so that the diameter of $T_{d,k}$ is *k*. Clearly the number of vertices of $T_{d,k}$ is given by $1 + \frac{d\left[(d-1)^k - 1\right]}{(d-2)}$, so that to obtain $T_{d,p}$ from $T_{d,p-1}$ we have to add $d(d-1)^{p-1}$ pendent vertices. Thus the number of vertices with distance from the centre v_0 as *p* is $d(d-1)^{p-1}$. For chemical relevance different topological indices of dendrimers has received lots of attention in both chemical as well as mathematical literature of which we only mention a few [7, 8, 9, 10].

In this paper, we derive some exact results for calculating the first and second reformulated Zagreb indices of dendrimers and also present some recurrence relations which calculate the and second reformulated Zagreb indices of bigger dendrimers in terms of smaller. Finally a relation between the first and second reformulated Zagreb indices is given.

2 Main Results

First we find an exact result which calculate the first reformulated Zagreb index of $T_{d,k}$.

Theorem 2.1. *The first reformulated Zagreb index of monocentric dendrimers* $T_{d,k}$ *is expressed as*

$$EM_1(T_{d,k}) = 4d(d-1)^2 \frac{(d-1)^{k-1} - 1}{d-2} + d(d-1)^{k+1} \qquad (1)$$

where, $d > 2$ *and* $k \geq 1$ *are any two integers.*

Proof. For $T_{d,k}$, we know that the degree of each non pendent vertices is d, so that $d(v_0) = d$, $d(v_{pj}) = d$ for $p = 1, 2, ..., k-1$ and $j = 1, 2, ..., d(d-1)^{(p-1)}$ and $d(v_{kj}) = d$ for $j = 1, 2, ..., d(d-1)^{(k-1)}$. Let us now denote the edges with one end vertex as degree one as pendent edge and others as non pendent edge so that the degree of each non pendent edge $2(d-1)$ and the degree of each pendent edge is

$(d-1)$. Also the number of edges with one end vertex v_0 is d and the number of edges with end vertices $v_{r,j}$ and $v_{r+1,q}$ (where $j=1,2,....,d(d-1)^{r-1}$ and $q=1,2,....,d(d-1)^{r}$) is given by $d(d-1)^{r-1}$ for $r=1,2,....,k-2$. So $T_{d,k}$ consists of $d(d-1)^{k-1}$ edges of degree $(d-1)$ and all the remaining edges are of degree $2(d-1)$. Thus the first reformulated Zagreb index of $T_{d,k}$ is given by

$$EM_1(T_{d,k}) = \sum_{e\in E(G)} d(e)^2 = 4d(d-1)^2\left[1+(d-1)+(d-1)^2+......+(d-1)^{(k-2)}\right]$$

$$+d(d-1)^{(k+1)} \quad (2)$$

$$= 4d(d-1)^2\sum_{i=0}^{k-2}(d-1)^i + d(d-1)^{(k+1)} = 4d(d-1)^2\frac{(d-1)^{k-1}-1}{d-2} + d(d-1)^{(k+1)}$$

from where the desired result follows. □

Now we find a recurrence relation between the first reformulated Zagreb index of $T_{d,k}$ and $T_{d,k+1}$.

Corollary 2.1. *The first reformulated Zagreb index of monocentric dendrimers* $T_{d,k}$ ($d>2$) *is recursively expressed as*

$$EM_1(T_{d,k+1}) = EM_1(T_{d,k}) + d(d-1)^{(k+1)}(d+2) \quad (3)$$

Proof. Again to find the recurrence relation, we can write from (2)

$$EM_1(T_{d,k+1}) = 4d(d-1)^2\sum_{i=0}^{k-1}(d-1)^i + d(d-1)^{(k+2)}$$

$$= 4d(d-1)^2\sum_{i=0}^{k-2}(d-1)^i + 4d(d-1)^{(k+1)} + d(d-1)^{(k+2)}$$

$$= EM_1(T_{d,k}) + 4d(d-1)^{k+1} + d(d-1)^{k+1}(d-2)$$

from where we get the desired recurrence relation. □

Next we calculate explicit formula to calculate second reformulated Zagreb index of $T_{d,k}$.

Theorem 2.2. *The second reformulated Zagreb index of monocentric dendrimers* $T_{d,k}$ *is expressed as*

$$EM_2(T_{d,k}) = \frac{1}{2}d(d-1)^{k+1}(d+6) \quad \text{for} \quad k>1 \quad (4)$$

and $EM_2(T_{d,k}) = 2d^2(d-1)^3$ *for* $k=1$*; ,where* $d>2$.

Proof. To calculate the second reformulated Zagreb index of $T_{d,k}$, we classify the edges of $T_{d,k}$ into following categories :

(i) First we consider the edges which are adjacent to v_0. The total number of pair of edges of this type is $\frac{d(d-1)}{2}$ and the degree of each edge of this type of edge is $2(d-1)$. Thus the contribution of these edges to the second reformulated Zagreb index is $2d(d-1)^3$.

(ii) Next we consider the edges of degree $2(d-1)$ connecting the vertices $v_{r,s}$ and $v_{r+1,t}$ where $r=1,2,....,k-2$; $s=1,2,....,d(d-1)^{r-1}$ and $t=1,2,....,d(d-1)^r$. Thus the contribution of these type of edges to the second reformulated Zagreb index is $2d(d-1)^3(d-2)(d-1)^{r-1}$ for $r=1,2,....,k-2$.

(iii) Now we consider the edges of degree $2(d-1)$ connecting the vertices $v_{k-2,s}$ and $v_{k-1,t}$ where $s=1,2,....,d(d-1)^{k-3}$ and $t=1,2,....,d(d-1)^{k-2}$ and the edges degree of *(d-1)* with end vertices $v_{k-1,j}$ and $v_{k,s}$ (for $j=1,2,....,d(d-1)^{k-2}$ and $s=1,2,....,d(d-1)^{k-1}$). The contribution of these edges to the second reformulated Zagreb index is $2(d-1)^2 d(d-1)^{k-1}$.

(iv) Lastly, for the edges with end vertices $v_{k-1,j}$ and $v_{k,s}$ (for $j=1,2,....,d(d-1)^{k-2}$ and $s=1,2,....,d(d-1)^{k-1}$) the degree of each edge is *(d-1)* and hence their contribution to the second reformulated Zagreb index is $\frac{d(d-2)(d-1)^{k+1}}{2}$.

Adding these contributions, the second reformulated Zagreb index of $T_{d,k}$ is given by

$$EM_2(T_{d,k}) = 2d(d-1)^3 + 2d(d-1)^3(d-2)\sum_{i=0}^{k-3}(d-1)^i + 2d(d-1)^{k+1} + \frac{1}{2}d(d-1)^{K+1}(d-2) \quad (5)$$

from where after some calculation we get the desired result.
If *k=1,* the desired result follows from the definition □

Similar to *Corollary 2.1* we now calculate relation between $EM_1(G)$ and $EM_2(G)$.

Corollary 2.2. *The second reformulated Zagreb index of* monocentric *dendrimers* $T_{d,k}$ *(* $d>2$ *) is recursively expressed as*

$$EM_2(T_{d,k+1}) = EM_2(T_{d,k}) + \frac{3}{2}d(d-2)(d-1)^{(k+1)} + \frac{1}{2}d(d+2)(d-1)^{k+2} - 2d(d-1)^{k+1} \quad (6)$$

Proof. Similar to *Corollary 2.1*, we can write from (5)

$$EM_2(T_{d,k+1}) = 2d(d-1)^3 + 2d(d-1)^3(d-2)\sum_{i=0}^{k-2}(d-1)^i + \frac{1}{2}d(d-2)(d-1)^{K+2} + 2d(d-1)^{k+2}$$

$$= 2d(d-1)^3 + 2d(d-1)^3(d-2)\sum_{i=0}^{k-3}(d-1)^i + 2d(d-1)^3(d-2)(d-1)^{k-2} + \frac{1}{2}d(d-2)(d-1)^{K+2}$$

$$+2d(d-1)^{k+2}$$

$$= EM_2(T_{d,k}) + 2d(d-1)^{k+1}(d-2) + \frac{1}{2}d(d-1)^{k+2}(d-2) + 2d(d-1)^{k+2} - \frac{1}{2}d(d-1)^{k+1}(d-2)$$

$$-2d(d-1)^{k+1}$$

from where after some calculation the desired recurrence relation follows. □

Now we establish a relation between first and second reformulated Zagreb index of Dendrimers $T_{d,k}$.

Theorem 2.2. *The first and second reformulated Zagreb index of monocentric dendrimers* $T_{d,k}$ *(* $d > 2, k > 1$ *) are related by*

$$EM_2(T_{d,k}) = \frac{1}{2}(d-1)(d-2)EM_1(T_{d,k}) + 2d(d-1)^3 - \frac{1}{2}d(d-1)^{k+2}(d-2) + \frac{1}{2}d(d-1)^{k+1}(10-3d)$$

Proof. To prove this theorem, from (2) we have

$$EM_1(T_{d,k}) = 4d(d-1)^2 S_1 + d(d-1)^{k+1} \tag{7}$$

where $S_1 = \sum_{i=0}^{k-2}(d-1)^i$. Similarly from (5) we can write

$$EM_2(T_{d,k}) = 2d(d-1)^3 + 2d(d-1)^3(d-2)S_1 - 2d(d-1)^{k+1}(d-2) + \frac{1}{2}d(d-1)^{k+1}(d-2) + 2d(d-1)^{K+1} \tag{8}$$

Now eliminating S_1 from (7) an (8), we have

$$EM_2(T_{d,k}) = \frac{1}{2}(d-1)(d-2)\left\{EM_1(T_{d,k}) - d(d-1)^{k+1}\right\} + 2d(d-1)^3 - \frac{1}{2}d(d-1)^{k+2}(d-2)$$

$$+\frac{1}{2}d(d-1)^{k+1}(10-3d)$$

from where the desired result follows. □

3 Conclusion

In this paper we the first and second reformulated Zagreb indices of a particular dendrimers is computed an hence some recurrence relations expressing bigger dendrimers in terms of smaller are given. Using these exact relations one can easily calculate the reformulated Zagreb indices of a particular dendrimers, for example, using relations (1) and (4) the first and second reformulated Zagreb indices of chemically important dendrimers $T_{3,k}$ are given by

$$EM_1(T_{3,k}) = 30.2^k - 48 \quad \text{and} \quad EM_2(T_{3,k}) = 27.2^k$$

for a fixed *k*. Using similar procedure, it is possible to calculate the reformulated Zagreb indices for other classes of dendrimers.

References

[1] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17, (1972), pp. 535-538.

[2] A. Milićević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, *Mol. Divers.* 8, (2004), pp. 393-399.

[3] G. Su, L. Xiong, L. Xu, B. Ma, On the maximum and minimum first reformulated Zagreb index with connectivity at most *k*, *Filomat*, 25, (2011), pp. 75-83.

[4] B. Zhou, N. Trinajstić, Some properties of the reformulated Zagreb indices, *J. Math. Chem.* 48, (2010), pp. 714-719.

[5] A. Ilić, B. Zhou, On reformulated Zagreb indices, Discrete Applied Mathematics 160, (2012), pp. 204-209.

[6] N. De, Some bounds of reformulated Zagreb indices, *Appl. Math. Sci.*, 6, No. 101-104, (2012), pp. 5005-5012.

[7] J. Yang, F. Xia, The Eccentric Connectivity Index of Dendrimers, *Int. J. Contemp. Math. Sciences,* 5(45), (2010), pp. 2231 -2236.

[8] N. De, Augmented Eccentric Connectivity Index of Some Thorn Graphs, *International Journal of Applied Mathematical Research*; Vol 1, No 4, (2012), pp. 671-680.

[9] H. Shabani, A. R. Ashrafi, M. V. Diudea, Balaban index of an infinite class of dendrimers, *Croat. Chem. Acta*, 83 (4), (2010), pp. 439–442.

[10] A. Madanshekaf, The Radníc index of some dendrimer nanostars, J. Appl. Math. & Informatics, 29, No. 5 - 6, (2011), pp. 1075 – 1080.

Received: February, 2013