ZAGREB INDICES OF A TREE WITH RADIUS 2

ABSTRACT

The first and second Zagreb index of a graph is defined as the sum of the squares of all vertices and sum of all product of the degrees of pairs of vertices respectively. These are degree based the topological indices. In this paper I calculated the first and second Zagreb indices of the graphs with radius two.

Keywords: *Topological Indices, Zagreb Indices, Chemical graph theory, Molecular structure*

Introduction:

Mathematical Chemistry was invented in the early 1980s to indicate the field that concerns itself with the new and nontrivial applications of mathematics to chemistry. Graph theory has been exploited for the solution of numerous practical problems, and it remain the same character. Chemical Graph theory has long and colorful history [4]. A molecular descriptor is the result of a logical and mathematical procedures which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment. The concept of molecular structure is one the most important concepts in the development of the scientific knowledge of the 20th century. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure [1,4].

In a graph G the diameter is defined [3]as

$$diam\ G = max_u max_v d(u,v)$$

And the radius of a Graph G is defined as

$$rad\ G = min_u max_v d(u,v)$$

the minimum and maximum distance is taken over all points u and v of G.

We can define these diameter and radius of a graph in terms of eccentricity also,

Let G = (V,E) be a graph and v be any vertex in G. The eccentricity $e(v)$ of a vertex v in G is defined to be

$$e(v) = max\{d(u,v)/u \in V\}$$

$$rad(G) = \min_{v\in V}\{ecc(v)\}$$

$$diam(G) = \max_{v\in V}\{ecc(v)\}$$

Philip A. Ostrand [3], established that $rad\ G \le diam\ G \le 2\ rad\ G$

Gutman, I[2], introduced the Zagreb indices in 1972. These indices are applied in QSAR/QSPR studies.

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The first Zagreb index $M_1(G)$ equal to the sum of squares of the degrees of the vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices of the underlying molecular graph G.

$$M_1(G) = \sum_{v \in V(G)} d(v)^2$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

Kinkar Ch. Das et.al., [9], obtained the lower and upper bound on the first Zagreb index $M_1(G)$ and Second Zagreb index $M_2(G)$ of G in terms of the number of vertices, edges, maximum vertex degree and minimum vertex degree. Also they have calculated the sum of the second Zagreb index and its complement of the graph.

Kexiang Xu [6], characterized the graph from $W_{n,k}$ with extremal Zagreb indices and determined the values of corresponding indices. P.S. Ranjini et.al., [10], investigated the Zagreb indices of the line graphs of the tadpole graphs, wheel graphs and ladder graphs using the subdivision concepts.

2.1.Lemma: Let T be a tree. Then

(1) the center of T is a vertex or two adjacent vertices,

(2) the center of T is one vertex if and only if $diam(T)$ =2rad(T).

The above two statements assert that if T is a tree of order n with the Zagreb ind among all trees of order at least five with radius two, then T has either one center or two adjacent vertices as centres. We denote by Tn,($n1$, . . . , nt) the tree of order n with radius two.

The unique center Vc such that (Vc) = t, (Vc) = {V1, . . . ,Vt}, and d(Vi) = ni + 1 for each i.

In particular, (n, t) =Tn,($n1$, . . . , nt), with $|ni - nj| \leq 1$ for any i, j.

2.2.Theorem : Let T = Tn,t($n1$, . . . , nt) be the tree as described[1]. Then the first and second Zagreb indices are $M_1\big(S(n,t)\big) = t^3 + 4t^2 + t$

$$M_2\big(S(n,t)\big) = nt(t+1) - t(t^3+1)$$

Proof: Here Total number of vertices, $n = 1 + t + t^2$,

Number of edges = $t^2 + t$

There are t number of vertices with (t+1) degree, t^2 number of vertices with degree 1 and 1 vertex which is a center vertex have degree t.

$$M_1\big(S(n,t)\big) = \sum_{v \in V(G)} d(v)^2$$
$$= t^2 + (t+1)^2 t + t^2(1)^2$$
$$M_1\big(S(n,t)\big) = t^3 + 4t^2 + t$$

$$M_2\big(S(n,t)\big) = \sum_{u,v \in V(G)} d(u)d(v)$$
$$= t[t(t+1)] + t^2[1.(t+1)]$$
$$M_2\big(S(n,t)\big) = 2t^2(t+1)$$

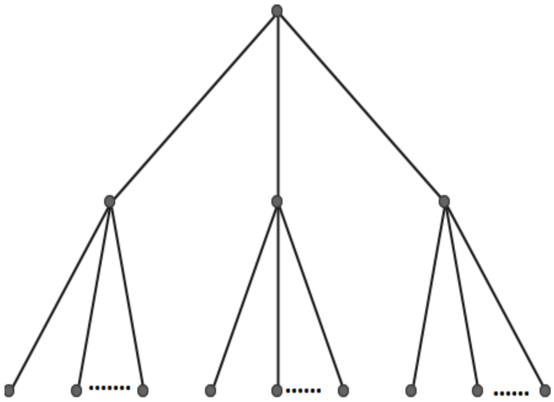

Fig.(1)

2.3.Theorem :

Let $T = T_{n,t+1}(n_1, \ldots, n_t)$ be the tree as described[1]. Then the first and second Zagreb indices are

$$M_1\big(S(n,t+1)\big) = t^3 + 3t^2 + t$$
$$M_2\big(S(n,t+1)\big) = t^3 + t^2$$

Proof:

Here Total number of vertices, $n = 1 + t + t^2$,

Number of edges = $t^2 + t$

There are (t+1) number of vertices with t degree, $t^2 - 1$ number of vertices with degree 1 and 1 vertex which is a center vertex have degree (t+1).

$$M_1\big(S(n,t+1)\big) = \sum_{v \in V(G)} d(v)^2$$
$$= (t+1)^2 + (t+1)t^2$$
$$+(t+1)(t-1)(1)^2$$
$$M_2\big(S(n,t+1)\big) = t^3 + 3t^2 + t$$

$$M_2\big(S(n,t+1)\big) = \sum_{u,v \in V(G)} d(u)d(v)$$

$$= t(t+1) + (t.1)(t-1)(t+1)$$

$$M_2\big(S(n,t+1)\big) = t^3 + t^2$$

Remark:

From the above two theorems we get the conclusion that

$$M_1\big(S(n,t)\big) \geq M_1\big(S(n,t+1)\big)$$

$$M_2\big(S(n,t)\big) \geq M_2\big(S(n,t+1)\big)$$

2.4. Corollary :

When $n \geq t + 2$, where n and t be two positive integers and

$1 + t + kt \leq n < 1 + t + (k+1)t$ for some integer $k \leq 0$ and $p = n - 1 - t - kt$ with degree 1.

$$M_1(G) = t^2 + (2p + k^2 + 3k + 1)t + p^2 + p$$

$$M_2(G) = kt^2 + (pk + p^2 + k^2 + k)t + p^2$$

Proof:

Total number of vertices, $n = 1 + t + t^2$,

Number of edges = $t + p + kt$

$$M_1(G) = (t+p)^2 + (k+1)^2 t + p(1)^2 + kt(1)^2$$

$$M_1(G) = t^2 + (2p + k^2 + 3k + 1)t + p^2 + p$$

$$M_2(G) = t[(t+p).k] + p[(t+p).1] + kt[(k+1).1]$$

$$M_2(G) = kt^2 + (pk + p^2 + k^2 + k)t + p^2$$

If $k = t$ and $p = 0$,

$$M_1(G) = M_1\big(S(n,t)\big)$$

$$M_2(G) = M_2\big(S(n,t)\big)$$

3. Theorem : If a tree T(n ,t) with two centers, then the Zagreb indices are

$M_1(G) = 2t^2 + 6t + 2$ and

$M_2(G) = 3t^2 + 4t + 1$

Proof:

Number of vertices in this graph $n = 2 + 2t$

Number of Edges $= 2t + 1$

In this tree there are 2 vertices have degree t+1 and 2t vertices have degree 1.

$$M_1(G) = 2(t+1)^2 + 2t(1)^2$$

$$M_1(G) = 2t^2 + 6t + 2$$

The second Zagreb index,

$M_2(G) = (t+1).(t+1) + (t+1).2t$

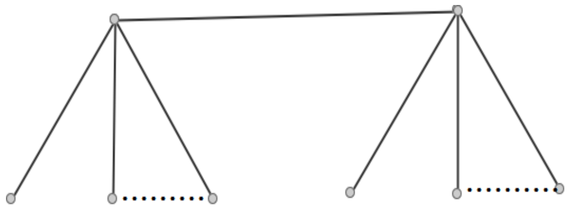

Fig.(2)

$$M_2(G) = 3t^2 + 4t + 1$$

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