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ZAGREB POLYNOMIALS AND MULTIPLE ZAGREB INDICES FOR COMB GRAPH

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Abstract

A topological index of graph G is a numerical parameter related to G, which characterizes its topology and is preserved under isomorphism of graphs. Properties of the chemical compounds and topological indices are correlated. In this report, we compute closed forms of first Zagreb, second Zagreb, first multiple Zagreb index and second multiple Zagreb index of comb graph. Moreover, we give graphical representation of our results, showing the dependence of our results on the involved structural parameters.

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1. Introduction

Chemical reaction network theory is an area of applied mathematics that attempts to model the behavior of real world chemical systems. Since its foundation in the 1960s, it has attracted a growing research community, mainly due to its applications in biochemistry and theoretical chemistry. It has also attracted interest from pure mathematicians due to the interesting problems that arise from the mathematical patterns in structures of material.

Cheminformatics is an emerging field in which quantitative structure-activity (QSAR) and structure-property (QSPR) relationships predict the biological activities and properties of nanomaterial. In these studies, some physico-chemical properties and topological indices are used to predict bioactivity of the chemical compounds [1-5].

The branch of chemistry which deals with the chemical structures with the help of mathematical tools is called *mathematical chemistry*. Chemical graph theory is the branch of mathematical chemistry that applies graph theory to mathematical modeling of chemical phenomena. In chemical graph theory, a molecular graph is a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges, respectively. A graph G with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a connection between any pair of vertices in G. The distance between two vertices u and v is denoted as $d(u, v)$ and is the length of shortest path between u and v in graph G. The number of vertices of G, adjacent to a given vertex v, is the "degree" of this vertex and will be denoted by $d(v)$. For details on the basics of graph theory, any standard text such as [6] can be of great help.

The first and the second Zagreb indices (cf. [7]) are defined as

$$M_1(G, x) = \sum_{uv \in E(G)} x^{[d(u)+d(v)]}, \quad M_2(G, x) = \sum_{uv \in E(G)} x^{[d(u)d(v)]}.$$

The multiplicative versions of the first and second Zagreb indices were first defined by Ghorbani and Azimi [8] as

$$PM_1(G) = \prod_{uv \in E(G)} [d(u) + d(v)] \quad \text{and} \quad PM_2(G) = \prod_{uv \in E(G)} [d(u)d(v)].$$

For details about chemical graph theory and topological indices, we refer the readers to [9, 10].

Let we have a path graph *P* of length *p*, if we attach *q* paths of length *r* at every vertex of degree two in *P*, we get comb graph $COM(p, q, r)$. In this paper, we compute the first and second Zagreb polynomials and first and second multiple Zagreb indices for the comb graph. A comb graph is shown in the following Figure 1:

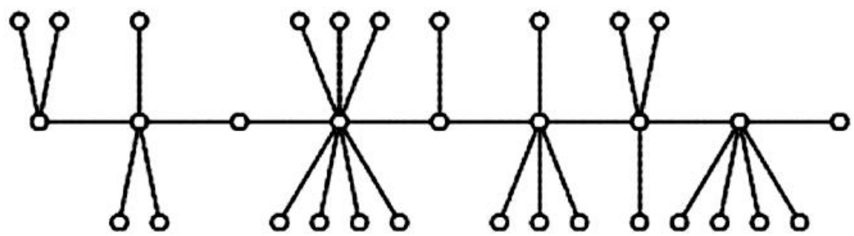

Figure 1. Comb graph.

2. Zagreb Polynomials

Let $COM(p, q, r)$ be the *comb graph*. One can observe that the $COM(p, q, r)$ has $q + pqr - npr$ number of vertices and $pqr - pr + q - 1$ number of edges. The vertex partition and edge partition of graph *G* are shown in Table 1 and Table 2, respectively.

Table 1. The vertex partition of comb graph

$d(v)$	1	2	$q+2$
Number of vertices	$2 + rq(p-2)$	$pr(q-2)$	$p-2$

Table 2. The edge partition of comb graph

$(d(u), d(v))$	$(1, 2)$	$(2, 2)$	$(1, q+2)$	$(q+2, q+2)$
Number of edges	$r(p-2)$	$(q-3)r(p-2)$	2	$p-3$

In this section, we will compute Zagreb polynomials and multiple Zagreb indices for the comb graph.

Theorem 2.1. *Let $COM(p, q, r)$ be the comb graph. Then*

$$M_1(COM(p, q, r), x) = r(p-2)x^3 + (q-3)r(p-2)x^4 + 2x^{q+3} + (p-3)x^{2q+4}.$$

Proof.

$$\begin{aligned} &M_1(COM(p, q, r), x) \\ &= \sum_{uv \in E(COM(p,q,r))} x^{[d(u)+d(v)]} \\ &= |E_1(COM(p, q, r))|x^3 + |E_2(COM(p, q, r))|x^4 \\ &\quad + |E_3(COM(p, q, r))|x^{q+3} + |E_4(COM(p, q, r))|x^{2q+4} \\ &= r(p-2)x^3 + (q-3)r(p-2)x^4 + 2x^{q+3} + (p-3)x^{2q+4}. \end{aligned}$$

Theorem 2.2. *Let $COM(p, q, r)$ be the comb graph. Then*

$$\begin{aligned} &M_2(COM(p, q, r), x) \\ &= r(p-2)x^2 + (q-3)r(p-2)x^4 + 2x^{q+2} + (p-3)x^{q^2+2q+4}. \end{aligned}$$

Proof.

$$\begin{aligned} &M_2(COM(p, q, r), x) \\ &= \sum_{uv \in E(COM(p,q,r))} x^{[d(u)d(v)]} \\ &= |E_1(COM(p, q, r))|x^2 + |E_2(COM(p, q, r))|x^4 + |E_3(COM(p, q, r))|x^{q+2} \\ &\quad + |E_4(COM(p, q, r))|x^{q^2+2q+4} \\ &= r(p-2)x^2 + (q-3)r(p-2)x^4 + 2x^{q+2} + (p-3)x^{q^2+2q+4}. \end{aligned}$$

3. Multiple Zagreb Indices

In this section, we compute multiple Zagreb indices for comb graph.

Theorem 3.1. *Let* $COM(p, q, r)$ *be the comb graph. Then*

$$PM_1(COM(p, q, r)) = 3^{r(p-2)}4^{r(p-2)(q-3)}(q+3)^2(2q+4)^{p-3}.$$

Proof.

$$PM_1(COM(p, q, r))$$

$$= \prod_{uv \in E(COM(p,q,r))} [d(u) + d(v)]$$

$$= 3^{|E_1(COM(p, q, r))|} \times 4^{|E_2(COM(p, q, r))|} \times (q+3)^{|E_3(COM(p, q, r))|}$$

$$\times (2q+4)^{|E_4(COM(p, q, r))|}$$

$$= 3^{r(p-2)}4^{r(p-2)(q-3)}(q+3)^2(2q+4)^{p-3}.$$

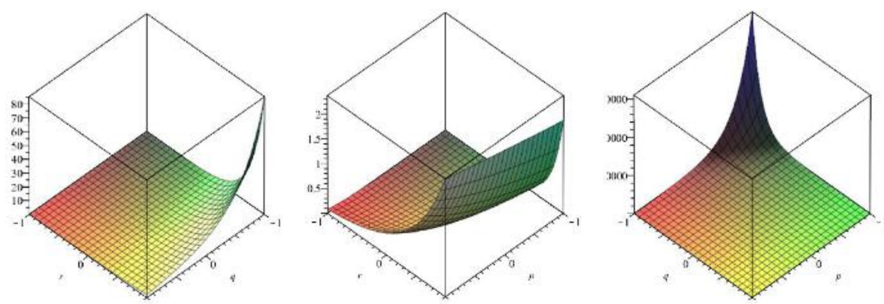

Figure 2. Plot of first multiplicative Zagreb index for $p = 1$ (left) for $q = 1$ (middle) for $r = 1$ (right).

Theorem 3.2. *Let* $COM(p, q, r)$ *be the comb graph. Then*

$$PM_2(COM(p, q, r)) = 2^{r(p-2)}4^{r(p-2)(q-3)}(q+2)^2(q^2+2q+4)^{p-3}.$$

Proof.

$$PM_2(COM(p, q, r))$$

$$= \prod_{uv \in E(COM(p,q,r))} [d(u)d(v)]$$

$$= 2^{|E_1(COM(p, q, r))|} \times 4^{|E_2(COM(p, q, r))|} \times (q+2)^{|E_3(COM(p, q, r))|}$$

$$\times (q^2 + 2q + 4)^{|E_4(COM(p, q, r))|}$$

$$= 2^{r(p-2)} 4^{r(p-2)(q-3)} (q+2)^2 (q^2 + 2q + 4)^{p-3}.$$

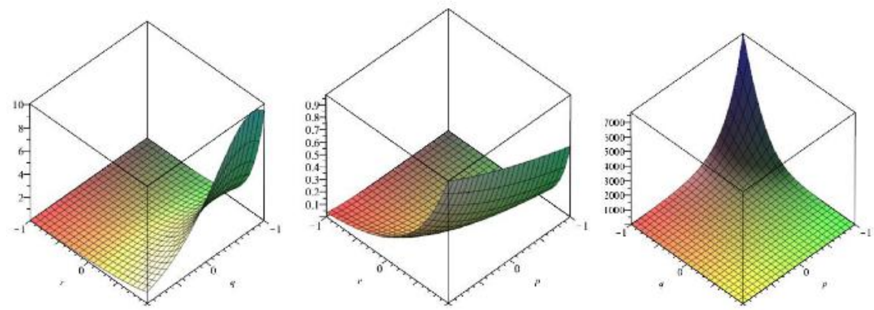

Figure 3. Plot of second multiple Zagreb index for $p = 1$ (left) for $q = 1$ (middle) for $r = 1$ (right).

References

[1] G. Rucker and C. Rucker, On topological indices, boiling points, and cycloalkanes, J. Chem. Inf. Comput. Sci. 39 (1999), 788-802.

[2] M. S. Sardar, S. Zafar and M. R. Farahani, The generalized Zagreb index of Capra-designed planar Benzenoid series $Ca_k(C_6)$, Open J. Math. Sci. 1(1) (2017), 44-51.

[3] H. M. ur Rehman, R. Sardar and R. Raza, Computing topological indices of Hex Board and its line graph, Open J. Math. Sci. 1(1) (2017), 62-71.

[4] N. De, Hyper Zagreb index of bridge and chain graphs, Open J. Math. Sci. 2(1) (2018), 1-17.

[5] W. Gao, B. Muzaffar and W. Nazeer, *K*-Banhatti and *K*-hyper Banhatti indices of dominating David derived network, Open J. Math. Anal. 1 (2017), 13-24.

[6] D. B. West, An Introduction to Graph Theory, Prentice-Hall, Englewood Cliffs, NJ, USA, 1996.

[7] I. Gutman and K. C. Das, The first Zagreb index 30 years after, MATCH-Commun. Math. Comput. Chem. 50 (2004), 83-92.

[8] M. Ghorbani and N. Azimi, Note on multiple Zagreb indices, Iran. J. Math. Chem. 3(2) (2012), 137-143.

[9] H. Siddiqui and M. R. Farahani, Forgotten polynomial and forgotten index of certain interconnection networks, Open J. Math. Anal. 1 (2017), 45-60.

[10] M. Riaz, W. Gao and A. Q. Baig, *M*-polynomials and degree-based topological indices of some families of convex polytopes, Open J. Math. Sci. 2(1) (2018), 18-28.