



On the Zagreb polynomials of graphs

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Abstract: First and second Zagreb polynomials are defined as $M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v}$ and $M_2 = \sum_{uv \in E(G)} x^{d_u} x^{d_v}$ respectively, where d_u is degree of vertex $u \in V(G)$ [1-3]. In this paper Zagreb polynomials of corona product of complete graphs, Zagreb polynomials of complement graph \bar{G} and Zagreb co-polynomials of graph G are studied.

Keywords: Complement graph, corona product of complete graph, Zagreb co-polynomial, Zagreb polynomial.

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I. Introduction

Let G be a simple, finite, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $u \in V(G)$ is denoted by d_u and is the number of vertices adjacent to u . The edge connecting the vertices u and v is denoted by uv . A molecular graph is presentation of the structural formula of a chemical compound in terms of graph theory whose vertices correspond to the atoms of compound and edges correspond to chemical bonds.

F-index of different products of graphs was studied by N.De [4]. Eccentric connectivity polynomial and total eccentricity polynomial of graph were studied in [5]. Different polynomials of molecular graphs were studied in [6-8]. Different versions of Gourava indices of Kragujevac tree networks were discussed by S.Kanwar et al. [9]. Novel harmonic indices of certain nanotubes were investigated by S.Ediz et al. [10]. Further studies on corona product of graphs can be found in [11-16]. Zagreb indices and Zagreb polynomials were studied [17-21]. Li Yan and W.Gao proposed eccentricity based fourth and sixth Zagreb polynomials in 2016 [22]. Distance based Wiener polynomial for corona product were studied in [23]. Motivated by the study of Zagreb indices and co-indices of molecular structure of methyl cyclopentane by K.Kiruthika [24], we take up investigation of Zagreb co-polynomials. In the mathematical field of graph theory a complete graph is a simple graph in which every pair of distinct vertices is connected by a unique edge, denoted by K_n , has n number of vertices and $\frac{n(n-1)}{2}$ number of edges. Let K_n and K_m be two complete graphs of order n and m . The edge partition for corona product is represented in table (1). The corona product of two graphs G and H is defined by taking one copy of G and $|V(G)|$ copies of H joining the i -th vertex G to every in the i -th copy of H [25]. The corona product is denoted by $G \odot H$. Zagreb polynomials of a graph G are defined and studied in [26-31]. The first Zagreb index of complement graph is defined as

$$M_1(\bar{G}) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u) + d_{\bar{G}}(v)}$$

$$= \sum_{uv \in E(\bar{G})} [n - 1 - d_G(u)] + [n - 1 - d_G(v)].$$

The complement of an edgeless graph is a complete graph and vice versa. In [32] the second hyper-Zagreb index of complement graph \bar{G} is defined as

$$HM_2(\bar{G}) = \sum_{uv \in E(\bar{G})} [\delta_{\bar{G}}(u) \delta_{\bar{G}}(v)]^2 = \sum_{uv \in E(\bar{G})} [n - 1 - \delta_G(u)]^2 [n - 1 - \delta_G(v)]^2.$$

The complement \bar{G} of a graph G is a graph whose vertex set is $V(G)$ and two vertices of \bar{G} are adjacent if and only if they are nonadjacent in G [33-35]. Therefore \bar{G} has n vertices and $\binom{n}{2} - m$ edges.

The degree of a vertex v in \bar{G} is $d_{\bar{G}}(v) = [n - 1 - d_G(v)]$. The Zagreb polynomials are defined as,

$$\text{first Zagreb polynomial: } M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v}$$

$$\text{second Zagreb polynomial: } M_2(G, x) = \sum_{uv \in E(G)} x^{d_u} x^{d_v},$$

$$\text{third Zagreb polynomial: } M_3(G, x) = \sum_{uv \in E(G)} x^{|d_u - d_v|},$$

$$\text{fourth Zagreb polynomial: } M_4(G, x) = \sum_{uv \in E(G)} x^{d_u(d_u + d_v)},$$

fifth Zagreb polynomial: $M_5(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v}$,
 general Zagreb polynomial: $M_{a,b}(G, x) = \sum_{uv \in E(G)} x^{(ad_u + bd_v)}$,
 and modified general Zagreb polynomial: $M'_{a,b}(G, x) = \sum_{uv \in E(G)} x^{(d_u + a)(d_v + b)}$.

We define Zagreb polynomials of a complement graph \bar{G} as,
 first Zagreb polynomial of \bar{G} : $M_1(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u) + d_{\bar{G}}(v)}$,
 second Zagreb polynomial of \bar{G} : $M_2(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u)d_{\bar{G}}(v)}$
 third Zagreb polynomial of \bar{G} : $M_3(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{|d_{\bar{G}}(u) - d_{\bar{G}}(v)|}$
 fourth Zagreb polynomial of \bar{G} : $M_4(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u)[d_{\bar{G}}(u) + d_{\bar{G}}(v)]}$
 fifth Zagreb polynomial of \bar{G} : $M_5(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(v)[d_{\bar{G}}(u) + d_{\bar{G}}(v)]}$
 general Zagreb polynomial of \bar{G} : $M_{a,b}(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{ad_{\bar{G}}(u) + bd_{\bar{G}}(v)}$
 and modified general Zagreb polynomial of \bar{G} : $M'_{a,b}(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{[d_{\bar{G}}(u) + a][d_{\bar{G}}(v) + b]}$

All the symbols and notations used in this paper are standard and taken from books of graph theory [36-38]. In this paper Zagreb polynomials of corona product and Zagreb polynomials of methyl cyclopentane are investigated.

II. Materials and Methods

A molecular graph $G(V, E)$ is constructed by representing each atom of molecule by vertex and bonds between them by edges. Let $V(G)$ be vertex set and $E(G)$ be edge set. The molecular graph of methyl cyclopentane is shown in figure 1. The degree of vertices in methyl cyclopentane is used to compute the Zagreb polynomials of complement graph and Zagreb co-polynomials. The complement graph \bar{G} of graph G is a graph whose vertex set is $V(G)$ and two vertices of \bar{G} are adjacent if and only if they are nonadjacent in G . A complete graph is a simple undirected graph in which every pair of distinct vertices is connected by a unique edge. The figure 2 represents corona product of complete graphs K_4 and K_3 . For Zagreb polynomials of complement graph, the proof follows from the definition of Zagreb polynomials and the degree of a vertex in the complement graph. The corona product of G and H is the graph $G \odot H$ obtained by taking one copy of G , called the center graph and $V(G)$ copies of H , called outer graph and making the i^{th} vertex of G adjacent to every vertex of the i^{th} copy of H , where i is $1 \leq i \leq |V(G)|$.

III. Results and Discussion

Let molecular graph of methyl cyclopentane is denoted by G . The expressions of Zagreb polynomial are used to compute Zagreb co-polynomial and Zagreb polynomial of complement graph. Other theorems can be obtained by using the corresponding expressions of Zagreb polynomial.

Theorem 1.1. First Zagreb polynomial of corona product of complete graphs K_n and K_m is

$$n \frac{m(m-1)}{2} x^{2m} + mn x^{2m+n-1} + \frac{n(n-1)^2}{2} x^{2(m+n-1)}.$$

Proof. By using definition and edge degree partition of corona product of complete graphs K_n and K_m , we get

$$\begin{aligned} \text{first Zagreb polynomial: } M_1(G_{K_n \odot K_m}, x) &= \sum_{uv \in E(G_{K_n \odot K_m})} x^{d_u + d_v} \\ &= \sum_{uv \in E_1} x^{m+m} + \sum_{uv \in E_2} x^{m+m+n-1} + \sum_{uv \in E_3} x^{m+n-1+m+n-1} \\ &= \sum_{uv \in E_1} x^{2m} + \sum_{uv \in E_2} x^{2m+n-1} + \sum_{uv \in E_3} x^{2(m+n-1)} \\ &= |E_1| x^{2m} + |E_2| x^{2m+n-1} + |E_3| x^{2(m+n-1)} \\ &= n \frac{m(m-1)}{2} x^{2m} + mn x^{2m+n-1} + \frac{n(n-1)^2}{2} x^{2(m+n-1)}. \end{aligned}$$

Theorem 1.2. Second Zagreb polynomial of corona product of complete graphs K_n and K_m is $n \left(\frac{m(m-1)}{2} \right) x^{m^2} + mn x^{m(m+n-1)} + \frac{n(n-1)}{2} x^{(m+n-1)^2}$.

Proof. By using definition and edge degree partition of corona product of complete graphs K_n and K_m we get

$$\begin{aligned} \text{second Zagreb polynomial: } M_2(G_{K_n \odot K_m}, x) &= \sum_{uv \in E(G_{K_n \odot K_m})} x^{d_u d_v} \\ &= \sum_{uv \in E_1} x^{m \cdot m} + \sum_{uv \in E_2} x^{m(m+n-1)} + \sum_{uv \in E_3} x^{(m+n-1)(m+n-1)} \\ &= |E_1| x^{m^2} + |E_2| x^{m(m+n-1)} + |E_3| x^{(m+n-1)(m+n-1)} \\ &= n \left(\frac{m(m-1)}{2} \right) x^{m^2} + mn x^{m(m+n-1)} + \frac{n(n-1)}{2} x^{(m+n-1)^2}. \end{aligned}$$

Theorem 1.3. Third Zagreb polynomial of corona product of complete graphs K_n and K_m is

$$n \left(\frac{m(m-1)}{2} \right) + mn x^{(n-1)} + \frac{n(n-1)}{2}.$$

Proof. By using definition and edge degree partition of corona product of complete graphs K_n and K_m , we get

$$\begin{aligned} \text{third Zagreb polynomial: } M_3(G_{K_n \odot K_m}, x) &= \sum_{uv \in E(G_{K_n \odot K_m})} x^{|d_u - d_v|} \\ &= \sum_{uv \in E_1} x^{|m - m|} + \sum_{uv \in E_2} x^{|m - (m+n-1)|} + \sum_{uv \in E_3} x^{|(m+n-1) - (m+n-1)|} \end{aligned}$$

$$= |E_1| + |E_2|x^{(n-1)} + |E_3|$$

$$= n\binom{m(m-1)}{2} + mnx^{(n-1)} + \frac{n(n-1)}{2}.$$

Theorem 1.4. Fourth Zagreb polynomial of corona product of complete graphs K_n and K_m is $n\binom{m(m-1)}{2}x^{2m^2} + mnx^{m(2m+n-1)} + \frac{n(n-1)}{2}x^{2(m+n-1)^2}$.

Proof. By using definitions and edge degree partition of corona product of complete graphs K_n and K_m , we get fourth Zagreb polynomial: $M_4(G_{K_n \odot K_m}, x) = \sum_{uv \in E(G_{K_n \odot K_m})} x^{d_u(d_u + d_v)}$

$$= \sum_{uv \in E_1} x^{m(m+m)} + \sum_{uv \in E_2} x^{m(m+(m+n-1))} + \sum_{uv \in E_3} x^{(m+n-1)[(m+n-1)+(m+n-1)]}$$

$$= |E_1|x^{m(m+m)} + |E_2|x^{m(2m+n-1)} + |E_3|x^{2[(m+n-1)(m+n-1)]}$$

$$= n\binom{m(m-1)}{2}x^{2m^2} + mnx^{m(2m+n-1)} + \frac{n(n-1)}{2}x^{2(m+n-1)^2}.$$

Theorem 1.5. Fifth Zagreb polynomial of corona product of complete graphs K_n and K_m is $n\binom{m(m-1)}{2}x^{2m^2} + mnx^{(m+n-1)(2m+n-1)} + \frac{n(n-1)}{2}x^{2(m+n-1)^2}$.

Theorem 1.6. Genral Zagreb polynomial of corona product of complete graphs K_n and K_m is $n\binom{m(m-1)}{2}x^{am+bm} + mnx^{am+b(m+n-1)} + \frac{n(n-1)}{2}x^{a(m+n-1)+b(m+n-1)}$.

Theorem 1.7. Modified general Zagreb polynomial of corona product of complete graphs K_n and K_m is $n\binom{m(m-1)}{2}x^{(m+a)(m+b)} + mnx^{(m+a)(m+n-1+b)} + \frac{n(n-1)}{2}x^{(m+n-1+a)+(m+n-1+b)}$.

Theorem 2.1. First Zagreb polynomial of complement graph \bar{G} is $x^7 + 3x^6 + 2x^5$.

Proof. By using definition and edge degree partition of \bar{G} , we get first Zagreb polynomial of \bar{G} : $M_1(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u) + d_{\bar{G}}(v)}$, where degree of a vertex v in \bar{G} is $d_{\bar{G}}(v) = [n - 1 - d_G(v)]$.

first Zagreb polynomial of \bar{G} : $M_1(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{[n-1-d_G(u) + (n-1-d_G(v))]}$

$$= x^7 + 3x^6 + 2x^5.$$

Theorem 2.2. Second Zagreb polynomial of complement graph \bar{G} is $x^{12} + 3x^9 + 2x^6$.

Proof. By using definition and edge degree partition of \bar{G} , we get second Zagreb polynomial of \bar{G} : $M_2(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u) d_{\bar{G}}(v)}$, where degree of a vertex v in \bar{G} is $d_{\bar{G}}(v) = [n - 1 - d_G(v)]$.

$M_2(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u) d_{\bar{G}}(v)} = \sum_{uv \in E(\bar{G})} x^{[n-1-d_G(u)][n-1-d_G(v)]}$

$$= \sum_{12 \in E_1} x^{(5-1)(5-2)} + \sum_{32 \in E_2} x^{(5-3)(5-2)} + \sum_{22 \in E_3} x^{(5-2)(5-2)}$$

$$= x^{12} + 3x^9 + 2x^6.$$

Theorem 2.3. Third Zagreb polynomial of complement graph \bar{G} is $3x+3$.

Proof. By using definition and edge degree partition of \bar{G} , we get third Zagreb polynomial of \bar{G} : $M_3(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{|d_{\bar{G}}(u) - d_{\bar{G}}(v)|} = \sum_{uv \in E(\bar{G})} x^{|[n-1-d_G(u)] - [n-1-d_G(v)]|}$

$$= \sum_{12 \in E_1} x^{|(5-1)-(5-2)|} + \sum_{32 \in E_2} x^{|(5-3)-(5-2)|} + \sum_{22 \in E_3} x^{|(5-2)-(5-2)|}$$

$$= 3x+3.$$

Theorem 2.4. Fourth Zagreb polynomial of complement graph \bar{G} is $x^{28} + 3x^{18} + 2x^{10}$.

Proof. By using definition and edge degree partition of molecular graph G , we get fourth Zagreb polynomial of \bar{G} : $M_4(\bar{G}, x) = \sum_{uv \in E(\bar{G})} x^{d_{\bar{G}}(u)[d_{\bar{G}}(u) + d_{\bar{G}}(v)]}$

$$= \sum_{12 \in E_1} x^{4[(5-1)+(5-2)]} + \sum_{32 \in E_2} x^{2[(5-3)+(5-2)]} + \sum_{22 \in E_3} x^{3[(5-2)+(5-2)]}$$

$$= x^{28} + 3x^{18} + 2x^{10}.$$

Theorem 2.5. Fifth Zagreb polynomial of complement graph \bar{G} is $x^{21} + 3x^{18} + 2x^{15}$.

Theorem 2.6. General Zagreb polynomial of complement graph \bar{G} is $x^{4a+3b} + 2x^{2a+3b} + 3x^{3a+3b}$.

Theorem 2.7. Modified general Zagreb polynomial of complement graph \bar{G} is $x^{(4+a)(3+b)} + 2x^{(2+a)(3+b)} + 3x^{(3+a)(3+b)}$.

Theorem 3.1. First Zagreb co-polynomial of graph G is $2x^5 + 3x^4 + 4x^3$.

Proof. By using definition and edge degree partition of molecular graph G , we get first Zagreb co-polynomial $\bar{M}_1(G, x) = \sum_{uv \notin E(G)} x^{d_u + d_v}$

$$= \sum_{uv \notin E_1} x^{d_u + d_v} + \sum_{uv \notin E_2} x^{d_u + d_v} + \sum_{uv \notin E_3} x^{d_u + d_v}$$

$$= \sum_{12 \notin E_1} x^{1+2} + \sum_{32 \notin E_2} x^{3+2} + \sum_{22 \notin E_3} x^{2+2}$$

$$= 2x^5 + 3x^4 + 4x^3.$$

Theorem 3.2. Second Zagreb co-polynomial of graph G is $2x^6 + 3x^4 + 4x^2$.

Proof. By using definition and edge degree partition of G , we get second Zagreb co-polynomial $\bar{M}_2(G, x) = \sum_{uv \notin E(G)} x^{d_u d_v}$

$$\begin{aligned}
 &= \sum_{uv \notin E_1} x^{d_u \cdot d_v} + \sum_{uv \notin E_2} x^{d_u \cdot d_v} + \sum_{uv \notin E_3} x^{d_u \cdot d_v} \\
 &= \sum_{12 \notin E_1} x^{1 \cdot 2} + \sum_{32 \notin E_2} x^{3 \cdot 2} + \sum_{22 \notin E_3} x^{2 \cdot 2} \\
 &= 2x^6 + 3x^4 + 4x^2.
 \end{aligned}$$

Theorem 3.3. Third Zagreb co-polynomial of graph G is $6x + 3$.

Proof. By using definition and edge degree partition of G, we get second Zagreb co-polynomial

$$\begin{aligned}
 \bar{M}_3(G, x) &= \sum_{uv \notin E(G)} x^{d_u \cdot d_v} \\
 &= \sum_{uv \notin E_1} x^{|d_u - d_v|} + \sum_{uv \notin E_2} x^{|d_u - d_v|} + \sum_{uv \notin E_3} x^{|d_u - d_v|} \\
 &= \sum_{12 \notin E_1} x^{|1-2|} + \sum_{32 \notin E_2} x^{|3-2|} + \sum_{22 \notin E_3} x^{|2-2|} \\
 &= 6x + 3.
 \end{aligned}$$

Theorem 3.4. Fourth Zagreb co-polynomial of graph G is $2x^{15} + 3x^8 + 4x^3$.

Proof. By using definitions and edge degree partition of G, we get fourth Zagreb co-polynomial

$$\begin{aligned}
 \bar{M}_4(G, x) &= \sum_{uv \notin E(G)} x^{d_u(d_u + d_v)} \\
 &= \sum_{uv \notin E_1} x^{d_u + d_v} + \sum_{uv \notin E_2} x^{d_u + d_v} + \sum_{uv \notin E_3} x^{d_u + d_v} \\
 &= \sum_{12 \notin E_1} x^{1(1+2)} + \sum_{32 \notin E_2} x^{3(3+2)} + \sum_{22 \notin E_3} x^{2(2+2)} \\
 &= 2x^{15} + 3x^8 + 4x^3.
 \end{aligned}$$

Theorem 3.5. Fifth Zagreb co-polynomial of graph G is $2x^{10} + 3x^8 + 4x^6$.

Theorem 3.6. General Zagreb co-polynomial of graph G is $4x^{a+2b} + 2x^{3a+2b} + 3x^{2a+2b}$.

Theorem 3.7. Modified general Zagreb co-polynomial of graph G is $4x^{(1+a)(2+b)} + 2x^{(3+a)(2+b)} + 3x^{(2+a)(2+b)}$.

Figure 1. The molecular graph of methyl cyclopentane and corona product of complement graphs K_4 and K_3 .

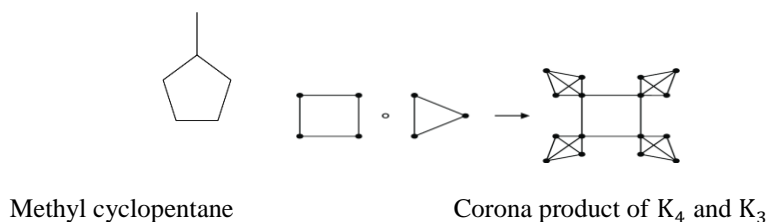


Table 1. The edge partition of corona product of complete graphs of order n and m based on degree set.

(d_u, d_v)	(m,m)	(m,m+n-1)	(m+n-1,m+n-1)
Number of edges	$\frac{m(m-1)}{2}$	mn	$\frac{n(n-1)}{2}$

IV. Conclusion

Zagreb polynomials of corona product of complete graphs, Zagreb polynomials of complement graph \bar{G} and Zagreb co-polynomials of graph G are obtained. Some Zagreb indices of methyl cyclopentane are $M_1(G) = 26, M_2(G) = 27, \bar{M}_1(G) = 34, \bar{M}_2(G) = 32, M_1(\bar{G}) = 56$ and $M_2(\bar{G}) = 87$.

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